Experimental study of the aqueous CO$_2$-NH$_3$ rate of reaction for temperatures from 15°C to 35°C, NH$_3$ concentrations from 5% to 15% and CO$_2$ loadings from 0.2 to 0.6

The absorption reaction between aqueous NH$_3$ and CO$_2$ was studied using the Wetted Wall Column. A total of 27 different cases are investigated in the region defined by temperatures from 15 °C to 35 °C, NH$_3$ concentrations from 5% to 15%, which are the typical solvent conditions in absorption columns, and lastly CO$_2$ loadings from 0.2 to 0.6. The resulting overall mass transfer coefficient of absorption measured follows the trends described by the modelling of the reactor and the equations used to describe the rate of the absorption reactions. Moreover, the overall mass transfer coefficient of absorption is in agreement with data available in the literature, valid in smaller portions of the investigated region. From the data analysis, the kinetics of the absorption reactions in the liquid phase is characterized. The equation proposed to fit the data is a power law equation which reproduces the experimental results measured at different CO$_2$ loadings. This represents a novelty because in literature the kinetic model of the reaction is usually fitted only to data for unloaded solutions (CO$_2$ loading equal to zero). Hence, in this case there is an experimental evidence that the kinetic model holds true in every loading conditions. The kinetic model intercept the values found in literature in every range of concentration. Consequently, the model is valid in every conditions and the rate of the reaction between NH$_3$ and CO$_2$ in liquid phase is described with an Arrhenius constant with a pre-exponential factor of $1.41 \times 10^{8}$ [mol/(m$^3$s)] and an activation energy of 60,680 [J/mol], a linear dependence on the CO$_2$ concentration and a dependence on the NH$_3$ with an exponent $\gamma = 1.89$. The proposed equation is found to be appropriate for implementation into process simulation software.
Influence of Adsorption and Capillary Pressure on Phase Equilibria Inside Shale Reservoirs

Due to the small pore sizes and organic content of shale, capillary pressure and adsorption are two effects that should be taken into account in the study of phase equilibrium inside shale. The inclusion of both effects in the phase equilibrium modeling can shed light on how bulk phase composition inside the porous media changes with temperature and pressure, and how the phase equilibrium changes accordingly. In the long run, such a model can be used in reservoir simulation for more complicated analysis. In this study, we present a calculation method that can effectively include adsorption and capillarity. We propose to introduce an excess adsorbed phase and treat the remaining substance inside the pores as a bulk phase (gas, liquid, or both) in order to make the mass balance formulation simpler. The adsorbed phase is modeled by the Multicomponent Langmuir (ML) equation for its simplicity and computational efficiency. A more theoretical adsorption model, the multicomponent potential theory of adsorption (MPTA), is used to determine the parameters of the simpler ML equation. The liquid and gas phases are described by the Peng-Robinson equation of state and the capillary pressure across their interface is taken into account. A flash algorithm by alternately updating the adsorbed phase amount and the fugacities in the bulk phases has been developed. The flash algorithm is used to analyze some representative systems (from binary, ternary to low-GOR and high-GOR model reservoir fluid systems) for the phase equilibrium inside porous media. The results show that adsorption and capillary pressure can significantly change the bulk phase composition and thus its corresponding phase envelope. Since the adsorption varies at different temperature and pressure conditions, the extent of change in the phase envelope is different. In general, a much shrunk phase envelope with a shifted critical point is observed. The heavier components are preferentially adsorbed in the whole pressure and temperature range studied here. At high pressure and low temperature, the selectivity towards heavier components is moderate in comparison to the that at low pressure and high temperature. The adsorption effects are stronger for the gas bulk phase region, leading to bigger changes in the gas phase composition and the shift of the dew point curve. PVT simulations of two model reservoir fluid systems show significant change in the results when capillary pressure and adsorption are included.

General information
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Organisations: Department of Chemistry, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Ressources Engineering, Center for Energy Resources Engineering
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Spectral/hp element methods: Recent developments, applications, and perspectives

The spectral/hp element method combines the geometric flexibility of the classical h-type finite element technique with the desirable numerical properties of spectral methods, employing high-degree piecewise polynomial basis functions on coarse finite element-type meshes. The spatial approximation is based upon orthogonal polynomials, such as Legendre or Chebychev polynomials, modified to accommodate a C0 - continuous expansion. Computationally and theoretically, by increasing the polynomial order p, high-precision solutions and fast convergence can be obtained and, in particular, under certain regularity assumptions an exponential reduction in approximation error between numerical and exact solutions can
be achieved. This method has now been applied in many simulation studies of both fundamental and practical engineering flows. This paper briefly describes the formulation of the spectral/hp element method and provides an overview of its application to computational fluid dynamics. In particular, it focuses on the use of the spectral/hp element method in transitional flows and ocean engineering. Finally, some of the major challenges to be overcome in order to use the spectral/hp element method in more complex science and engineering applications are discussed.

**General information**
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Organisations: Department of Applied Mathematics and Computer Science, Scientific Computing, Center for Energy Resources Engineering, Technical University of Denmark, Imperial College London, Aalborg University
Authors: Xu, H. (Ekstern), Cantwell, C. (Ekstern), Monteserin, C. (Ekstern), Eskilsson, C. (Ekstern), Engsig-Karup, A. P. (Intern), Sherwin, S. (Ekstern)
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Scopus rating (2015): SJR 0.252 SNIP 0.393 CiteScore 1.24
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Scopus rating (2007): SJR 0.208 SNIP 0.66
Scopus rating (2006): SJR 0.247 SNIP 1.208
Scopus rating (2005): SJR 0.199 SNIP 0.842
Scopus rating (2004): SJR 0.202 SNIP 0.74
Scopus rating (2003): SJR 0.2 SNIP 0.304
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The Debye-Hückel theory and its importance in modeling electrolyte solutions

A colleague at the Technical University of Denmark has often stated: “Life is too short for electrolytes”. Another well-known scientist in the field of molecular simulation has recently said during an international Thermodynamics conference: “All my life I have tried to keep myself away from water and electrolytes”. Sadly, what these statements correctly imply is that there are far too many unclear questions and concepts in electrolyte thermodynamics, and associated difficulties in modeling electrolyte solutions. In this work, we attempt to shed some light on some important concepts and misconceptions in electrolyte thermodynamics associated with the development of electrolyte equations of state, with emphasis on those based on the Debye-Hückel theory. Detailed mathematics is needed for some of the derivations but for brevity and in order to emphasize the principles rather than the derivations, the latter are omitted. We first discuss the peculiarities of electrolyte thermodynamics and associated modeling and continue with the derivation of the Debye-Hückel theory. The assumptions and limits of application of Debye-Hückel are discussed in particular. Next, the Born term and its significance and implications are presented in more detail. A discussion and outlook section conclude this review. Several of the statements in this work challenge “accepted beliefs” in electrolyte thermodynamics and, while we believe that this challenge is justified, we hope that a useful debate can result in improved and predictive thermodynamic models for electrolyte solutions.

General information
State: Accepted/In press
Organisations: Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Ressources Engineering, KT Consortium
Authors: Kontogeorgis, G. M. (Intern), Maribo-Mogensen, B. (Intern), Thomsen, K. (Intern)
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Web of Science (2017): Indexed yes
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Scopus rating (2016): CiteScore 2.33 SJR 0.869 SNIP 1.155
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BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.874 SNIP 0.998 CiteScore 1.99
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 0.982 SNIP 1.248 CiteScore 2.28
Web of Science (2014): Indexed yes
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Scopus rating (2013): SJR 1.007 SNIP 1.274 CiteScore 2.31
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
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Scopus rating (2012): SJR 1.152 SNIP 1.286 CiteScore 2.31
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.034 SNIP 1.234 CiteScore 2.26
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 0.986 SNIP 1.317
Web of Science (2010): Indexed yes
17th International Conference on Petroleum Phase Behavior and Fouling

This special section of Energy & Fuels contains contributed papers from the 17th International Conference on Petroleum Phase Behavior and Fouling (Petrophase 2016). Petrophase 2016 was organized by the Technical University of Denmark and Schlumberger and took place in Elsinore (Helsingør) Denmark from June 19th to 23rd at the Beach Hotel Marienlyst. Petrophase is an international conference aimed at researchers in industry and academia dedicated to the study of the properties and chemistry of petroleum fluids and their effect on producing, processing, and refining in the upstream, midstream, and downstream industries. The conference started in 1999 as "The International Conference on Petroleum Phase Behavior & Fouling" and has since evolved into an annual event taking place in countries all around the world. Petrophase has been fortunate to have enjoyed financial and organizational support from many academic and industrial institutions through the years. Despite its growth over the years, Petrophase has always had the feel of an intimate conference where all participants are present in all of the activities.

General information
State: Published
Organisations: Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering, Department of Chemistry, Asphaltam
Authors: von Solms, N. (Intern), Yan, W. (Intern), Andersen, S. (Ekstern)
Pages: 3329-3329
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Main Research Area: Technical/natural sciences

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Journal: Energy and Fuels
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Adaptive control in an artificial pancreas for people with type 1 diabetes

In this paper, we discuss overnight blood glucose stabilization in patients with type 1 diabetes using a Model Predictive Controller (MPC). We compute the model parameters in the MPC using a simple and systematic method based on a priori available patient information. We describe and compare 3 different model structures. The first model structure is an autoregressive integrated moving average with exogenous input (ARIMAX) structure. The second model structure is an autoregressive moving average with exogenous input (ARMAX) model, i.e. a model without an integrator. The third model structure is an adaptive ARMAX model in which we use a recursive extended least squares (RELS) method to estimate parameters of the stochastic part. In addition, we describe some safety layers in the control algorithm that improve the controller robustness and reduce the risk of hypoglycemia. We test and compare our control strategies using a virtual clinic of 100 randomly generated patients with a representative inter-subject variability. This virtual clinic is based on the Hovorka model. We consider the case where only half of the meal bolus is administered at mealtime, and the case where the insulin sensitivity increases during the night. The numerical results suggest that the use of an integrator leads to higher
occurrence of hypoglycemia than for the controllers without the integrator. Compared to other control strategies, the adaptive MPC reduces both the time spent in hypoglycemia and the time spent in hyperglycemia.
A least squares approach for efficient and reliable short-term versus long-term optimization

The uncertainties related to long-term forecasts of oil prices impose significant financial risk on ventures of oil production. To minimize risk, oil companies are inclined to maximize profit over short-term horizons ranging from months to a few years. In contrast, conventional production optimization maximizes long-term profits over horizons that span more than a decade. To address this challenge, the oil literature has introduced short-term versus long-term optimization. Ideally, this problem is solved by a posteriori multi-objective optimization methods that generate an approximation to the Pareto front of optimal short-term and long-term trade-offs. However, such methods rely on a large number of reservoir simulations and scale poorly with the number of objectives subject to optimization. Consequently, the large-scale nature of production optimization severely limits applications to real-life scenarios. More practical alternatives include ad hoc hierarchical switching schemes. As a drawback, such methods lack robustness due to unclear convergence properties and do not naturally generalize to cases of more than two objectives. Also, as this paper shows, the hierarchical formulation may skew the balance between the objectives, leaving an unfulfilled potential to increase profits. To promote efficient and reliable short-term versus long-term optimization, this paper introduces a natural way to characterize desirable Pareto points and proposes a novel least squares (LS) method. Unlike hierarchical approaches, the method is guaranteed to converge to a Pareto optimal point. Also, the LS method is designed to properly balance multiple objectives, independently of Pareto front’s shape. As such, the method poses a practical alternative to a posteriori methods in situations where the frontier is intractable to generate.
An algorithm for gradient-based dynamic optimization of UV flash processes

This paper presents a novel single-shooting algorithm for gradient-based solution of optimal control problems with vapor-liquid equilibrium constraints. Such optimal control problems are important in several engineering applications, for instance in control of distillation columns, in certain two-phase flow problems, and in operation of oil reservoirs. The single-shooting algorithm uses an adjoint method for the computation of gradients. Furthermore, the algorithm uses either a simultaneous or a nested approach for the numerical solution of the dynamic vapor-liquid equilibrium model equations. Two numerical examples illustrate that the simultaneous approach is faster than the nested approach and that the efficiency of the underlying thermodynamic computations is important for the overall performance of the single-shooting algorithm. We compare the performance of different optimization software as well as the performance of different compilers in a Linux operating system. These tests indicate that real-time nonlinear model predictive control of UV flash processes is computationally feasible.

General information
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Organisations: Center for Energy Resources Engineering, Department of Applied Mathematics and Computer Science, Scientific Computing
Authors: Ritschel, T. K. S. (Intern), Capolei, A. (Intern), Gaspar, J. (Intern), Jørgensen, J. B. (Intern)
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Journal: Computers & Chemical Engineering
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BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
An efficient and rigorous thermodynamic library and optimal-control of a cryogenic air separation unit

Cryogenic air separation (CAS) is the leading technology for large scale production of pure N2, O2 and Ar. This process is very electric-energy intensive; thus it is a likely candidate for load balancing of power stations in a smart grid. This type of intermittent operation of CAS, requires a non-linear model based control to achieve optimal techno-economic
performance. Accordingly, this work presents a computationally efficient and novel approach for solving a tray-by-tray equilibrium model and its implementation for open-loop optimal-control of a cryogenic distillation column. Here, the optimisation objective is to reduce the cost of compression in a volatile electricity market while meeting the production requirements, i.e. product flow rate and purity. This model is implemented in Matlab and uses the ThermoLib rigorous thermodynamic library. The present work represents a first step towards plant-wide dynamic modelling and smart control of a cryogenic distillation plant.

General information
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Organisations: Department of Applied Mathematics and Computer Science, Scientific Computing, Center for Energy Resources Engineering
Authors: Gaspar, J. (Intern), Ritschel, T. K. S. (Intern), Jørgensen, J. B. (Intern)
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Cryogenic air separation, Load balancing, Distillation column, Dynamic modeling, Optimal-control
DOIs: 10.1016/B978-0-444-63965-3.50259-2
Publication: Research - peer-review › Article in proceedings – Annual report year: 2017

A Novel Approach for Risk Minimization in Life-Cycle Oil Production Optimization
The oil research community has invested much effort into computer aided optimization to enhance oil recovery. While simulation studies have demonstrated the potential of model-based technology to improve industrial standards, the largely unknown geology of subsurface reservoirs limits applications to commercial oil fields. In particular, uncertain model descriptions lead to risks of profit loss. To address the challenges of geological uncertainty, this paper proposes offset risk minimization. As opposed to existing methodologies of the oil literature, the offset approach minimizes risk of profit loss relative to industrial standards. A numerical case study compares the offset approach to a representative selection of current state-of-the-art methodologies. The results show that the offset approach offers the overall lowest risk of profit loss relative to industrial best practices. This suggests that it may be more relevant to consider offset risk minimization than conventional ensemble-based methods for the purpose of life-cycle production optimization

General information
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Organisations: Department of Applied Mathematics and Computer Science, Center for Energy Resources Engineering, Scientific Computing
Authors: Capolei, A. (Intern), Christiansen, L. H. (Intern), Jørgensen, J. B. (Intern)
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Optimal control of oil reservoirs, Risk management, Stochastic modelling
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A Riccati-Based Interior Point Method for Efficient Model Predictive Control of SISO Systems
This paper presents an algorithm for Model Predictive Control of SISO systems. Based on a quadratic objective in addition to (hard) input constraints it features soft upper as well as lower constraints on the output and an input rate-of-change penalty term. It keeps the deterministic and stochastic model parts separate. The controller is designed based on the
A Thermodynamic Library for Simulation and Optimization of Dynamic Processes

Process system tools, such as simulation and optimization of dynamic systems, are widely used in the process industries for development of operational strategies and control for process systems. These tools rely on thermodynamic models and many thermodynamic models have been developed for different compounds and mixtures. However, rigorous thermodynamic models are generally computationally intensive and not available as open-source libraries for process simulation and optimization. In this paper, we describe the application of a novel open-source rigorous thermodynamic library, ThermoLib, which is designed for dynamic simulation and optimization of vapor-liquid processes. ThermoLib is implemented in Matlab and C and uses cubic equations of state to compute vapor and liquid phase thermodynamic properties. The novelty of ThermoLib is that it provides analytical first and second order derivatives. These derivatives are needed for efficient dynamic simulation and optimization. The analytical derivatives improve the computational performance by a factor between 12 and 35 as compared to finite difference approximations. We present two examples that use ThermoLib routines in their implementations: (1) simulation of a vapor-compression cycle, and (2) optimal control of an isoenergetic-isochoric flash separation process. The ThermoLib software used in this paper is distributed as open-source software at www.psetools.org.
Can smartphone-based electronic markers discriminate between patients with bipolar disorder, healthy first-degree relatives and healthy control individuals

General information
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Organisations: Copenhagen Center for Health Technology, Department of Applied Mathematics and Computer Science, Cognitive Systems, Center for Energy Resources Engineering, Embedded Systems Engineering
Authors: Stanislaus, S. (Ekstern), Faurholt-Jepsen, M. (Ekstern), Vinberg, M. (Ekstern), Winther, O. (Intern), Frost, M. G. (Intern), Bardram, J. E. (Intern), Kessing, L. (Ekstern)
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Comparison of GERG-2008 and simpler EoS models in calculation of phase equilibrium and physical properties of natural gas related systems

Accurate description of thermodynamic properties of natural gas systems is of great significance in the oil and gas industry. For this application, non-cubic equations of state (EoSs) are advantageous due to their better density and compressibility description. Among the non-cubic models, GERG-2008 is a new wide-range EoS for natural gases and other mixtures of 21 natural gas components. It is considered as a standard reference equation suitable for natural gas applications where highly accurate thermodynamic properties are required. Soave's modification of Benedict-Webb-Rubin (Soave-BWR) EoS is another model that despite its empirical nature, provides accurate density description even around the critical point. It is much simpler than GERG-2008 and easier to handle and generalize to reservoir oil fluids. This study presents a comprehensive comparison between GERG-2008 and other cubic (SRK and PR) and noncubic EoSs (Soave-BWR and PC-SAFT) with a focus on Soave-BWR in description of pure components density and compressibility in a wide temperature and pressure range, calculation of binary Vapor-Liquid-Equilibria (VLE) and density, prediction of multicomponent phase envelopes and gas compressibility factor. In addition, the performance of GERG-2008 is compared with that of cubic and non-cubic models in calculation of thermal properties such as heat capacity and Joule-Thomson coefficient for pure components and multicomponent mixtures over a wide pressure and temperature range. The results are compared with available experimental data in the literature and special emphasis has been given to the reverse Joule-Thomson effects at high pressure high temperature (HPHT) conditions. © 2016 Elsevier B.V. All rights reserved.
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
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Web of Science (2016): Indexed yes
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Scopus rating (2015): SJR 0.874 SNIP 0.998 CiteScore 1.99
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BFI (2014): BFI-level 2
Scopus rating (2014): SJR 0.982 SNIP 1.248 CiteScore 2.28
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Scopus rating (2013): SJR 1.007 SNIP 1.274 CiteScore 2.31
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
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Scopus rating (2012): SJR 1.152 SNIP 1.286 CiteScore 2.31
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.034 SNIP 1.234 CiteScore 2.26
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
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Scopus rating (2010): SJR 0.986 SNIP 1.317
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Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.227 SNIP 1.09
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.031 SNIP 1.151
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Web of Science (2005): Indexed yes
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Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 0.722 SNIP 1.101
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 0.966 SNIP 1.284
Web of Science (2001): Indexed yes
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Web of Science (2000): Indexed yes
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10.1016/j.fluid.2016.11.016
Source: PublicationPreSubmission
Source-ID: 127460058
**Complete mitochondrial genome of the Oriental Hornet, Vespa orientalis F. (Hymenoptera: Vespidae)**

The Oriental Hornet (Vespa orientalis) is a social insect belonging to the Vespiade family (Wasps, Hornets, Yellowjackets), genus Vespa (true Hornets). The oriental hornet is a scavenger and an agricultural pest, especially to bee farmers, but is also recently described as a harvester of solar energy. Here, we report the mitochondrial genome sequence of the Oriental Hornet, Vespa orientalis F., which may play a vital role in understanding this wasp biology, light trapping and generation of electricity. The mitochondrial genome of this hornet is 16,099 bp in length, containing 13 protein-coding genes, 21 transfer RNA genes, and 2 ribosomal RNA genes. The overall base composition of the heavy-strand is 40.3% A, 5.9% C, 13.2% G, and 40.6% T, the percentages of A and T being higher than that of G and C. The mitochondrial genome of the Oriental Hornet, Vespa orientalis F. represents the first mitogenome of a solar energy harvesting insect.

**General information**

State: Published
Organisations: Department of Bio and Health Informatics, Metagenomics, Center for Energy Resources Engineering, CERE – Center for Energy Resources Engineering, National Center for Agricultural Research and Extension, Swedish Museum of Natural History
Authors: Haddad, N. J. (Ekstern), Al-Nakeeb, K. A. A. (Intern), Petersen, B. (Intern), Dalén, L. (Ekstern), Sorgenfrei Blom, N. (Intern), Sicheritz-Pontén, T. (Intern)
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Publication: Research - peer-review » Journal article – Annual report year: 2017

**Complex conductivity of soils**

The complex conductivity of soil remains poorly known despite the growing importance of this method in hydrogeophysics. In order to fill this gap of knowledge, we investigate the complex conductivity of 71 soils samples (including 4 peat samples) and one clean sand in the frequency range 0.1 Hertz to 45 kHz. The soil samples are saturated with 6 different NaCl brines with conductivities (0.031, 0.53, 1.15, 5.7, 14.7, and 22 S m⁻¹, NaCl, 25°C) in order to determine their intrinsic formation factor and surface conductivity. This dataset is used to test the predictions of the dynamic Stern polarization model of porous media in terms of relationship between the quadrature conductivity and the surface conductivity. We also investigate the relationship between the normalized chargeability (the difference of in phase conductivity between two frequencies) and the quadrature conductivity at the geometric mean frequency. This dataset confirms the relationships between the surface conductivity, the quadrature conductivity, and the normalized chargeability. The normalized chargeability depends linearly on the cation exchange capacity and specific surface area while the chargeability shows no dependence on these parameters. These new data and the dynamic Stern layer polarization model are observed to be mutually consistent. Traditionally, in hydrogeophysics, surface conductivity is neglected in the analysis of resistivity data. The relationships we have developed can be used in field conditions to avoid neglecting surface conductivity in the interpretation of DC resistivity tomograms. We also investigate the effects of temperature and saturation and, here again, the dynamic Stern layer predictions and the experimental observations are mutually consistent.

**General information**
Computation of Phase Equilibrium and Phase Envelopes

In this technical report, we describe the computation of phase equilibrium and phase envelopes based on expressions for the fugacity coefficients. We derive those expressions from the residual Gibbs energy. We consider 1) ideal gases and liquids modeled with correlations from the DIPPR database and 2) nonideal gases and liquids modeled with cubic equations of state. Next, we derive the equilibrium conditions for an isothermal-isobaric (constant temperature, constant pressure) vapor-liquid equilibrium process (PT flash), and we present a method for the computation of phase envelopes. We formulate the involved equations in terms of the fugacity coefficients. We present expressions for the first-order derivatives. Such derivatives are necessary in computationally efficient gradient-based methods for solving the vapor-liquid equilibrium equations and for computing phase envelopes. Finally, we describe a Matlab program that computes the phase envelope of a mixture. We present the source code and discuss practical details of the implementation.

General information

State: Published
Organisations: Department of Applied Mathematics and Computer Science, Scientific Computing, Center for Energy Resources Engineering
Authors: Ritschel, T. K. S. (Intern), Jørgensen, J. B. (Intern)
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tr17_11_Ritschel_TKS.pdf
Publication: Research - peer-review › Report – Annual report year: 2017

Controls on Cementation in a Chalk Reservoir

In this study, we identify different controls on cementation in a chalk reservoir. Biot's coefficient, a measure of cementation, stiffness and strength in porous rocks, is calculated from logging data (bulk density and sonic P-wave velocity). We show that Biot's coefficient is correlated to the water saturation of the Kraka reservoir and is partly controlled by its stratigraphic sub-units. While the direct causal relationship between Biot's coefficient and water saturation cannot be extended for Biot's coefficient and porosity, a correlation is also identified between the two, implying that some degree of pore filling cementation occurred in Kraka (Alam, 2010). Lack of correlation between Biot's coefficient and Gamma Ray (GR) indicates that the small amount of clay present is generally located in the pore space, thus not contributing to frame stiffness. While there was no compositional control on cementation via clay, we could infer that stratigraphy impacts on the diagenetic process.
Seasonal storage of excess heat in hot deep aquifers is considered to optimize the usage of commonly available energy sources. The chemical effects of heating the Gassum Sandstone Formation to up to 150 degrees C is investigated by combining laboratory core flooding experiments with petrographic analysis and geochemical modeling. Synthetic formation water is injected into two sets of Gassum Formation samples at 25, 50 (reservoir temperature), 100, and 150 degrees C with a velocity of 0.05 and 0.1 PV/h, respectively. Results show a significant increase in the aqueous concentration of silicium and iron with increasing temperature due to dissolution of silica and siderite. Increasing the reservoir temperature from 50 to 100 degrees C enhanced the naturally occurring weathering of Na-rich feldspar to kaolinite. Dissolution of quartz increased sharply above 100 degrees C and was the dominating process at 150 degrees C, resulting in a significant increase in the aqueous silicium concentration. At temperatures, 100 degrees C, the silicium concentration was controlled by a quasi-stationary state between feldspar dissolution and kaolinite precipitation whereas the concentration was kinetically controlled by quartz dissolution at 150 degrees C. Furthermore, a strong coupling between dissolution, precipitation, and flow velocity was observed. The results of this study show that the effects of heat storage of up to 150 degrees C in the Gassum Formation in the Stenlille area is expected to have only minor effects on the properties of the reservoir and that storage of excess heat in the Gassum Formation in the Stenlille area may be possible provided operational precautions are taken.

Cross-Validation of a Glucose-Insulin-Glucagon Pharmacodynamics Model for Simulation using Data from Patients with Type 1 Diabetes

Background:
Currently, no consensus exists on a model describing endogenous glucose production (EGP) as a function of glucagon concentrations. Reliable simulations to determine the glucagon dose preventing or treating hypoglycemia or to tune a
dual-hormone artificial pancreas control algorithm need a validated glucoregulatory model including the effect of glucagon.

Methods:
Eight type 1 diabetes (T1D) patients each received a subcutaneous (SC) bolus of insulin on four study days to induce mild hypoglycemia followed by a SC bolus of saline or 100, 200, or 300 µg of glucagon. Blood samples were analyzed for concentrations of glucagon, insulin, and glucose. We fitted pharmacokinetic (PK) models to insulin and glucagon data using maximum likelihood and maximum a posteriori estimation methods. Similarly, we fitted a pharmacodynamic (PD) model to glucose data. The PD model included multiplicative effects of insulin and glucagon on EGP. Bias and precision of PD model test fits were assessed by mean predictive error (MPE) and mean absolute predictive error (MAPE).

Results:
Assuming constant variables in a subject across nonoutlier visits and using thresholds of ±15% MPE and 20% MAPE, we accepted at least one and at most three PD model test fits in each of the seven subjects. Thus, we successfully validated the PD model by leave-one-out cross-validation in seven out of eight T1D patients.

Conclusions:
The PD model accurately simulates glucose excursions based on plasma insulin and glucagon concentrations. The reported PK/PD model including equations and fitted parameters allows for in silico experiments that may help improve diabetes treatment involving glucagon for prevention of hypoglycemia.
Data Requirements and Modeling for Gas Hydrate-Related Mixtures and a Comparison of Two Association Models

The association theory-based advanced thermodynamic models have gained more and more attention and applications in many industries. The cubic plus association (CPA) and the simplified perturbed chain statistical associating fluid theory (sPC-SAFT) equations of state (EOS) are two of the most widely used association models in the chemical and petroleum industries. The CPA model is extensively used in flow assurance, in which the gas hydrate formation is one of the central topics. Experimental data play a vital role in validating models and obtaining model parameters. In this work, we will compare the performance of the CPA and sPC-SAFT EOS for modeling the fluid-phase equilibria of gas hydrate-related systems and will try to explore how the models can help in suggesting experimental measurements. These systems contain water, hydrocarbon (alkane or aromatic), and either methanol or monoethylene glycol. It is well known that the determination of SAFT-type model parameters for associating fluids remains a challenge because there are at least five pure-component parameters for these compounds and there is no property combination found to be enough to ensure the best parameter set. Therefore, in this work two parameter sets have been chosen for the sPC-SAFT EOS for a fair comparison. The comparisons are made for pure fluid properties, vapor liquid-equilibria, and liquid liquid equilibria of binary and ternary mixtures as well as vapor liquid liquid equilibria of quaternary mixtures. The results show, from an overall point of view, that these two models have equally good performance, and the two parameter sets with the sPC-SAFT EOS are also comparable, especially for the vapor liquid equilibria systems. Moreover, the modeling results suggest that some data are less reliable than others, which indicates the need for more measurements to further validate the models, especially for multicomponent systems.

General information
State: Published
Organisations: Center for Energy Resources Engineering, Centre for oil and gas – DTU, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering, KT Consortium, Technical University of Denmark
Authors: Liang, X. (Intern), Aloupis, G. (Ekstern), Kontogeorgis, G. M. (Intern)
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Web of Science (2018): Indexed yes
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Web of Science (2017): Indexed Yes
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Scopus rating (2016): CiteScore 2.29 SJR 0.88 SNIP 1.097
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.868 SNIP 0.966 CiteScore 1.96
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.021 SNIP 1.208 CiteScore 2.22
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
A new experimental set-up and methodology for the measurement of ZnS solubility in aqueous solutions at 40, 60 and 80 °C (atmospheric pressure) is presented. The methodology implemented includes the preparation of the samples in a reduced oxygen atmosphere, particle size analysis of ZnS, quality control of the analytical technique and evaluation of equilibration time. ZnS solubility analyses were run for prolonged times (up to 11 days) to ensure that equilibrium conditions were met. The equilibration time was explored at three temperatures (40, 60 and 80 °C) observing small variations in the time required to reach the solid–liquid equilibrium at each temperature. Equilibrium was reached within 72 h. The concentration of zinc and of total sulfur were determined using Inductively Coupled Plasma Optical Emission Spectroscopy (ICP-OES). The experimental solubility data show an exponential dependency of the solubility with respect to temperature. An increase of 40 °C results in an increase of roughly 12 times for the solubility of ZnS.

**General information**

State: Published
Organisations: Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering, Department of Chemistry
Dynamic Optimization of UV Flash Processes

UV ash processes, also referred to as isoenergetic-isochoric ash processes, occur for dynamic simulation and optimization of vapor-liquid equilibrium processes. Dynamic optimization and nonlinear model predictive control of distillation columns, certain two-phase ow problems, as well as oil reservoirs with signi cant compositional and thermal e ects may be conducted as dynamic optimization of UV ash processes. The dynamic optimization problem involving a UV ash problem is formulated as a bilevel optimization problem. This problem is solved using a gradient based single-shooting method. The gradients are computed using the adjoint method and different o -the-shelf optimization software (fmincon, IPOPT, KNITRO, NPSOL) are used for the numerical optimization. Computational results are reported for a ash process involving benzene, toluene and diphenyl. The computational experiments demonstrate that the optimization solver, the compiler, and high-performance linear algebra software are all important for e cient dynamic optimization of UV ash processes.

General information
State: Published
Organisations: Center for Energy Resources Engineering, Department of Applied Mathematics and Computer Science, Scientific Computing
Authors: Ritschel, T. K. S. (Intern), Capolei, A. (Intern), Jørgensen, J. B. (Intern)
Number of pages: 6
Publication date: 2017

Economic Optimizing Control for Single-Cell Protein Production in a U-Loop Reactor

The production of single-cell protein (SCP) in a U-loop reactor by a methanotroph is a cost efficient sustainable alternative to protein from fish meal obtained by over-fishing the oceans. SCP serves as animal feed. In this paper, we present a mathematical model that describes the dynamics of SCP production in a U-loop reactor. We use this model to compute an optimal start-up trajectory by solution of an economic optimizing optimal control problem. The optimal start-up trajectory is an unstable attractor. The practical implementation of this optimal start-up trajectory can be conducted by a proportional controller for the substrate concentration in the top tank of the U-loop reactor.

General information
State: Published
Organisations: Department of Applied Mathematics and Computer Science, Scientific Computing, Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, PROSYS - Process and Systems Engineering Centre, Centre for oil and gas – DTU, Technical University of Denmark
Authors: Drejer, A. (Ekstern), Ritschel, T. K. S. (Intern), Jørgensen, S. B. (Intern), Jørgensen, J. B. (Intern)
Pages: 1759-1764
Publication date: 2017
**eCPA: An ion-specific approach to parametrization**

Abstract The eCPA equation of state has been shown to be a promising electrolyte model, for which several applications have been demonstrated. The model at its current status is, however, limited by the use of salt-specific parameters for the interactions between salts and water. Having salt-specific parameters limit the applicability to simple systems of ions, as it can only be applied when a common ion is found between the salts in the solution. For more complex systems of multiple ions/salts this may not work well. In this work the main goal is to eliminate this limitation by parametrizing the model with an ion-specific parameter set. The ion-specific parameters are estimated by a simultaneous fitting of parameters for 17 ions, consisting of 10 cations and 7 anions, and with data for 55 salts. The parameters are fitted to osmotic coefficient and mean ionic activity coefficient data in a wide temperature range from 273.15K to above 500K and up to an ionic strength of 6 molal. The parameters are found to yield similar deviations as the salt-specific parameters, however, for a few salts cation-anion interaction parameters were needed in order to obtain reasonable accuracy. The parameters are applied to a series of systems, which include mixed salt osmotic coefficients, solid-liquid equilibrium and vapor-liquid equilibrium of water-methanol-salt, illustrating the applicability of the ion-specific parameters. Modelling of mixed salt osmotic coefficients illustrate that the parameters work well in salt mixtures, while the phase equilibria also illustrate the extension to mixed solvent systems.

**General information**

State: Accepted/In press  
Organisations: Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering, Center for Energy Resources Engineering, KT Consortium  
Authors: Schlaikjer, A. (Intern), Thomsen, K. (Intern), Kontogeorgis, G. M. (Intern)  
Number of pages: 15  
Publication date: 2017  
Main Research Area: Technical/natural sciences

**Publication information**

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Web of Science (2017): Indexed yes  
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Scopus rating (2016): CiteScore 2.33 SJR 0.869 SNIP 1.155  
Web of Science (2016): Indexed yes  
BFI (2015): BFI-level 2  
Scopus rating (2015): SJR 0.874 SNIP 0.998 CiteScore 1.99  
Web of Science (2015): Indexed yes  
BFI (2014): BFI-level 2  
Scopus rating (2014): SJR 0.982 SNIP 1.248 CiteScore 2.28  
Web of Science (2014): Indexed yes  
BFI (2013): BFI-level 2  
Scopus rating (2013): SJR 1.007 SNIP 1.274 CiteScore 2.31  
ISI indexed (2013): ISI indexed yes  
Web of Science (2013): Indexed yes  
BFI (2012): BFI-level 2  
Scopus rating (2012): SJR 1.152 SNIP 1.286 CiteScore 2.31  
ISI indexed (2012): ISI indexed yes  
Web of Science (2012): Indexed yes  
BFI (2011): BFI-level 2  
Scopus rating (2011): SJR 1.034 SNIP 1.234 CiteScore 2.26  
ISI indexed (2011): ISI indexed yes  
Web of Science (2011): Indexed yes  
BFI (2010): BFI-level 2  
Scopus rating (2010): SJR 0.986 SNIP 1.317  
Web of Science (2010): Indexed yes
Effective stresses and shear failure pressure from in situ Biot's coefficient, Hejre Field, North Sea: Stresses and shear failure pressure

We propose a combination of Biot's equations for effective stress and the expression for shear failure in a rock to obtain an expression for minimum pore pressure in a stable vertical well bore. We show that a Biot's coefficient calculated from logging data in the Hejre Field, North Sea, is significantly different from 1. The log-derived Biot's coefficient is above 0.8 in the Shetland Chalk Group and in the Tyne Group, and 0.6-0.8 in the Heno Sandstone Formation. We show that the effective vertical and horizontal stresses obtained using the log-derived Biot's coefficient result in a drilling window for a vertical well larger than if approximating Biot's coefficient by 1. The estimation of the Biot's coefficient is straightforward in formations with a stiff frame, whereas in formations such as shales, caution has to be taken. We discuss the consequence of assumptions made on the mineral composition of shales as unphysical results could be obtained when choosing inappropriate mineral moduli.

General information
State: Published
Organisations: Department of Civil Engineering, Section for Geotechnics and Geology, Center for Energy Resources Engineering, DONG Energy AS
Authors: Regel, J. B. (Intern), Orozova-Bekkevold, I. (Intern), Andreassen, K. A. (Intern), van Gilse, N. C. H. (Ekstern), Fabricius, I. L. (Intern)
Number of pages: 15
Pages: 808-822
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Geophysical Prospecting
Volume: 65
Issue number: 3
ISSN (Print): 0016-8025
Ratings:
Elasticity and Density of Paleozoic Shales from Bornholm
The Paleozoic shales exposed on the island of Bornholm contain intervals with more than 10% organic matter which is post mature with respect to the formation of hydrocarbons. Four shallow bore holes have been drilled through the 250 m thick shale interval and partly cored and logged with geophysical probes. We studied how the organic content and mineralogical composition influence mass density and elastic properties as measured from core analysis and logging data. The shales have porosity in the range of 1%-10% and modelled permeability (from porosity and BET) of generally less
than 0.1 μDarcy. We found that solid density and elastic stiffness parameters only vary insignificantly with solid composition, when TOC is lower than 5%, but that mass density and TOC are correlated when TOC is higher than 5%. A similar correlation was not seen for TOC and Sonic logging data. A reason can be that the content of low-density kerogen and high-density pyrite is correlated. According to our data, the shales have weak to medium degree anisotropy of stiffness and compare well with other studied shales.

**General information**

State: Published

Organisations: Department of Civil Engineering, Section for Geotechnics and Geology, Center for Energy Resources Engineering, Technical University of Denmark, Geological Survey of Denmark and Greenland

Authors: Fabricius, I. L. (Intern), Haugwitz, C. (Ekstern), Larsen, P. B. (Intern), Schovsbo, N. (Ekstern)

Number of pages: 8

Pages: 1299-1306

Publication date: 2017

**Host publication information**

Title of host publication: Poromechanics 2017 - Proceedings of the 6th Biot Conference on Poromechanics

Publisher: American Society of Civil Engineers

ISBN (Electronic): 978-078448077-9

Main Research Area: Technical/natural sciences


DOIs: 10.1061/9780784480779.161

Publication: Research - peer-review › Article in proceedings – Annual report year: 2017

**Electrical Double-Layer and Ion Bridging Forces between Symmetric and Asymmetric Charged Surfaces in the Presence of Mono- and Divalent Ions**

An atomic force microscope, employing the colloidal probe technique, was used to study the interactions between six different combinations of silane-functionalized silica surfaces in NaCl and CaCl₂ solutions. The surfaces consisted of monolayers of the apolar trimethoxy(octyl)silane, the positively charged (3-aminopropyl)trimethoxysilane, and the negatively charged (3-mercaptopropyl)trimethoxysilane. The interactions between the three symmetric systems, as well as between the three asymmetric combinations of surfaces, were measured and compared to calculated electrical double-layer forces. The results demonstrated that the long-range interactions between the surfaces in all cases were dominated by double-layer forces, while short-range interactions, including adhesion, were dominated by ion bridging forces in the cases where both interaction surfaces favored adsorption of calcium ions. The study thus also demonstrates how surface force studies in mono- and divalent salt solutions can be used as an analytical tool for probing specific functional groups on heterogeneous surfaces.

**General information**

State: Published

Organisations: Department of Chemistry, Centre for oil and gas – DTU, Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering

Authors: Liu, X. (Intern), Feilberg, K. L. (Intern), Yan, W. (Intern), Stenby, E. H. (Intern), Thormann, E. (Intern)

Number of pages: 9

Pages: 4426-4434

Publication date: 2017

Main Research Area: Technical/natural sciences

**Publication information**

Journal: Langmuir

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Issue number: 18

ISSN (Print): 0743-7463

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Web of Science (2017): Indexed Yes

BFI (2016): BFI-level 2

Scopus rating (2016): CiteScore 3.99 SJR 1.55 SNIP 1.188

Web of Science (2016): Indexed yes

BFI (2015): BFI-level 2

Scopus rating (2015): SJR 1.686 SNIP 1.308 CiteScore 4.33
Flooding of North Sea chalk and greensand cores with specific brines

General information
State: Published
Organisations: Department of Civil Engineering, Section for Geotechnics and Geology, Center for Energy Resources Engineering, CERE – Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, Department of Chemistry
General approach to characterizing reservoir fluids for EoS models using a large PVT database

Fluid characterization is needed when applying any EoS model to reservoir fluids. It is important especially for non-cubic models such as PC-SAFT where fluid characterization is less mature. Furthermore, there is a great interest to apply non-cubic models to high pressure high temperature reservoir fluids as they are believed to give better description of density and compressibility over a wide temperature and pressure range. We proposed a general approach to characterizing reservoir fluids and applied it to PC-SAFT. The approach consists in first, developing the correlations based on the DIPPR database, and then adjusting the correlations based on a large PVT database. The adjustment was made to minimize the deviation in key PVT properties like saturation pressures, densities at reservoir temperature and stock tank oil densities, while keeping the n-alkane limit of the correlations unchanged. The general approach can also be applied to other EoS models for improving their fluid characterization and we showed this for SRK and PR. In addition, we developed a PNA based characterization method for PC-SAFT based on the same general principles. We made a comprehensive comparison in PVT calculation involving 17 EoS-characterization combinations and 260 reservoir fluids. The new characterization methods generally improved the PVT calculation results.

General information
State: Published
Organisations: Department of Chemistry, Center for Energy Resources Engineering, CERE – Center for Energy Resources Engineering
Authors: Varzandeh, F. (Intern), Stenby, E. H. (Intern), Yan, W. (Intern)
Number of pages: 15
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Main Research Area: Technical/natural sciences
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Journal: Fluid Phase Equilibria
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Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Helbredstjek af dansk sundhedsteknologi: Sektorudviklingsrapport
Sådan kan samarbejde mellem industrien, universiteterne og sundhedsvæsenet skabe gode løsninger til forebyggelse, diagnostik, patientbehandling og rehabilitering

General information
State: Published
Organisations: Office for Innovation & Sector Services, Copenhagen Center for Health Technology, Department of Applied Mathematics and Computer Science, Embedded Systems Engineering, Center for Energy Resources Engineering, Scientific Computing, Department of Management Engineering, Technology and Innovation Management, Department of Electrical Engineering, Biomedical Engineering, Department of Bio Integrated Systems, Department of Photonics Engineering, Diode Lasers and LED Systems, Department of Energy Conversion and Storage, Electrofunctional materials, IT Service, National Space Institute, Innovation and Research-based consultancy, Department of Chemical and Biochemical Engineering, The Danish Polymer Centre, Office for Research and Relations, It-branchen, manjourn.dk
Number of pages: 72
Publication date: 2017

High pressure phase equilibrium of ternary and multicomponent alkane mixtures in the temperature range from (283–473) K
Asymmetric multicomponent alkane mixtures can be used as model systems for reservoir fluids. We have prepared two ternary mixtures, methane/n-butane/n-decane and methane/n-butane/n-dodecane, and two multicomponent mixtures composed of methane/n-butane/n-octane/n-dodecane/n-hexadecane/n-eicosane as model reservoir fluids and measured their phase equilibrium in the temperature range from (283–473) K by using a variable volume cell with full visibility. Their phase envelopes and liquid volume fractions below the saturation pressure have been measured. Four equations of state, including Soave-Redlich-Kwong (SRK), Peng-Robinson (PR), Perturbed Chain Statistical Associating Fluid Theory (PC-SAFT), and Soave-Benedict-Webb-Rubin (Soave-BWR), have been used to predict phase equilibrium of the measured systems. PR and PC-SAFT give better results than others and Soave-BWR gives poor phase envelope predictions which are quite distinct from the predictions by other models. It is generally challenging for any of the tested models to predict all the measured phase envelopes with high accuracy. For predictive calculation of the liquid fractions, the agreement in the low pressure region is good whereas the fractions just below the saturation pressures are difficult to predict. Moreover GERG-2008 has also been tested with the measured methane/n-butane/n-decane system. It over predicts the saturation pressures but predicts low pressure liquid fractions quite accurately.

General information
State: Published
Organisations: Center for Energy Resources Engineering, Department of Chemistry, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Ressources Engineering, Technical University of Denmark
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BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 2.33 SJR 0.869 SNIP 1.155
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.874 SNIP 0.998 CiteScore 1.99
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 0.982 SNIP 1.248 CiteScore 2.28
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.007 SNIP 1.274 CiteScore 2.31
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.152 SNIP 1.286 CiteScore 2.31
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.034 SNIP 1.234 CiteScore 2.26
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 0.986 SNIP 1.317
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.133 SNIP 1.164
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.227 SNIP 1.09
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.031 SNIP 1.151
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.034 SNIP 1.245
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.009 SNIP 1.3
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 0.985 SNIP 1.349
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 1.193 SNIP 1.301
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 0.722 SNIP 1.101
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 0.966 SNIP 1.284
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 0.87 SNIP 0.898
Web of Science (2000): Indexed yes
Scopus rating (1999): SJR 0.938 SNIP 0.885
Original language: English
n-alkanes mixture, Phase equilibrium, Liquid fraction, High pressure, High Temperature
DOIs: 10.1016/j.fluid.2017.06.021
High Pressure Rheological Behavior of 1-Ethyl-3-methylimidazolium n-Hexylsulfate and Trihexyl(tetradecyl)phosphonium Tris(pentafluoroethyl)trifluorophosphate

Ionic liquids have been broadly studied in the past decade for being used as lubricants or lubricant additives. The rheological characterization of these fluids is very important in this context because it determines to a great extent their performance for different lubricants applications, such as hydraulic or gear lubricants. Thus, in this work we have performed the rheometric characterization of two ionic liquids (ILs), 1-ethyl-3-methylimidazolium n-hexylsulfate and trihexyl(tetradecyl)phosphonium tris(pentafluoroethyl)trifluorophosphate, in the temperature range from 298.15 to 353.15 K up to 75 MPa and shear rates up to 1000 s⁻¹. For this aim, the setup of a new device for rheological characterization at high pressure based on Couette flow and concentric cylinders was undertaken in this work. Moreover the pressure–viscosity and temperature–viscosity coefficients of these ILs have been calculated. Both ILs present Newtonian behavior in the studied conditions. The trifluorophosphate IL has strong pressure–viscosity dependence, whereas for the other IL this dependence is quite slight.

General information
State: Published
Organisations: Center for Energy Resources Engineering, Department of Chemistry, Department of Chemical and Biochemical Engineering, University of Santiago de Compostela, University of Vigo
Authors: Regueira, T. (Intern), Lugo, L. (Ekstern), Comuñas, M. J. P. (Ekstern), Fernández, J. (Ekstern)
Pages: 2927-2936
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Scopus rating (2016): CiteScore 2.29 SJR 0.88 SNIP 1.097
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.868 SNIP 0.966 CiteScore 1.96
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.021 SNIP 1.208 CiteScore 2.22
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.135 SNIP 1.199 CiteScore 2.17
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.141 SNIP 1.103 CiteScore 2.01
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.862 SNIP 0.988 CiteScore 1.8
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.054 SNIP 1.299
Induced Shear Failure by Temperature Reduction at Uni-axial Strain Conditions

General information
State: Published
Organisations: Department of Civil Engineering, Section for Geotechnics and Geology, Center for Energy Resources Engineering, University of Stavanger
Authors: Voake, T. (Ekstern), Nermoen, A. (Ekstern), Korsnes, R. (Ekstern), Fabricius, I. L. (Intern)
Number of pages: 11
Publication date: 2017
Main Research Area: Technical/natural sciences
Electronic versions: Untitled.pdf
Source: PublicationPreSubmission
Source-ID: 140684882
Publication: Research - peer-review › Paper – Annual report year: 2017

Low-Field NMR Spectrometry of Chalk and Argillaceous Sandstones: Rock-Fluid Affinity Assessed from T-1/T-2 Ratio
Nuclear magnetic resonance (NMR) procedure typically minimizes the effects of external magnetic field gradients on the transverse relaxation. Thus, longitudinal, and transverse, T-2, relaxation times should in principle be similar. However, internal magnetic field gradients related to minerals can shorten T-2, as compared to provided the saturating fluid has high affinity to the solid. Consequently, the T-1/T-2 ratio should quantify the affinity between the mineral and wetting pore fluid, so we estimate wettability from logging data by comparing the T-1/T-2 ratio of oil and water peaks in the reservoir zone to the T-1/T-2 ratio in the water zone. We tested the hypothesis on core samples and used the predicted wettability to successfully determining the elastic bulk modulus of samples containing oil and water.
In order to investigate the T-2-shortening, we performed 1D and 2D NMR experiments on samples of chalk, kaolinitic sandstone, and chloritic greensand, saturated either with water, oil or oil/water at irreducible water saturation. The 1D NMR experiment involved determination of T-2 spectrum, whereas the 2D NMR experiments included determination of T-1-T-2 and D-T-2 maps, where D is the intrinsic diffusion coefficient.T-2 spectra show that in all water-saturated samples, surface relaxation dominates; in oil-saturated chalk and kaolinitic sandstone, bulk relaxation dominates; whereas T-2 of oil-saturated greensand shows surface relaxation in the part of the spectrum representing chlorite. In all samples with irreducible water
saturation, water shows surface relaxation, whereas oil shows bulk relaxation. In line with this observation, D-T-2 maps of these samples show field gradient effects in the oil, but not in the water indicating that the water is trapped between solid and oil due to restricted diffusion. A T-2 shortening will increase the T-1/T-2 ratio, so we use the T-1/T-2 ratio obtained from T-1-T-2 maps as a measure of fluid-mineral affinity. By this measure, the chalk shows high affinity for water, the kaolinitic sandstone has no clear preference for oil or water, whereas chloritic greensand shows different behavior for small and large pores. Small pores (fast-relaxing components) have T-1/T-2 = 2.0 when water saturated, but T-1/T-2 = 3.8 when oil saturated, indicating oil-affinity of chlorite. By contrast, large pores (slow-relaxing components) have significant preference for water (T-1/T-2 = 2.2) as compared to oil (T-1/T-2 = 1.2 to 1.4). Overall, this paper provides an insight into the preference of a mineral to a fluid and ultimately into determining the wettability and correct pore-fluid distribution of a reservoir rock.

**General information**

State: Published  
Organisations: Department of Civil Engineering, Section for Geotechnics and Geology, Center for Energy Resources Engineering, Colorado School of Mines  
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Scopus rating (2007): SJR 0.371 SNIP 0.543  
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Scopus rating (2005): SJR 0.471 SNIP 0.886  
Scopus rating (2004): SJR 0.579 SNIP 1.423  
Scopus rating (2003): SJR 0.341 SNIP 0.872  
Scopus rating (2002): SJR 0.323 SNIP 0.391  
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Low field NMR surface relaxivity studies of chalk and argillaceous sandstones

This paper addresses how the surface relaxivity, $\rho$, of rock forming minerals as assessed from low field Nuclear Magnetic Resonance (NMR) spectrometry, is affected by temperature and Larmor frequency. This is relevant for connecting laboratory data and reservoir logging data while increasing the accuracy of predictions of petrophysical properties of various rocks with the use of NMR spectrometry. We perform laboratory transverse relaxation ($T_2$) measurements on water saturated Gorm field chalk, Stevns Klint chalk, Solsort field greensand and Berea sandstone. These rocks are of particular interest in studies related to the North Sea oil and gas reservoirs, since they cover a wide range of formations, ranging from homogeneous to inhomogeneous chalk, chloritic and quartz mineralogy. Comparison of $T_2$ distributions at Larmor frequency of 2 and 20 MHz at 40 °C shows that paramagnetic minerals in the Gorm field chalk and Solsort field greensand have higher $\rho$ at higher Larmor frequency. By contrast, $\rho$ of the purely calcitic Stevns chalk and quartzitic Berea sandstone proved not to be affected by the changes in frequency. $T_2$ distributions at temperatures ranging from 10 °C to 60 °C provided comparison between lab and field $T_2$ measurements: $\rho$ for calcite decreases with temperature; whereas $\rho$ for quartz increases with temperature. These findings illustrate differences in the porosity and pore size distribution obtained in the lab, compared to those from logs using NMR tools.
Modeling Pharmacokinetics and Pharmacodynamics of Glucagon for Simulation of the Glucoregulatory System in Patients with Type 1 Diabetes.

The goal of this thesis was to develop a pharmacokinetics/pharmacodynamics (PK/PD) model for glucagon. The proposed PD model included multiplication of the stimulating glucagon effect and inhibiting insulin effect on the endogenous glucose production (EGP). Moreover, the concentration-response relationship of glucagon and EGP was characterized by a nonlinear function, where the response saturated for high concentrations of glucagon. The novel EGP model extended Hovorka's glucoregulatory model to include the effect of glucagon. The PK/PD model described both regular glucagon and a novel glucagon analogue in healthy dogs. The extended glucoregulatory model translated to the human species and described glucose-insulin-glucagon dynamics in healthy subjects and patients with type 1 diabetes (T1D). The extended glucoregulatory model was successfully validated by leave-one-out cross-validation in seven T1D patients which justified its use for simulations. The final model parameters were estimated from three to four datasets from each patient. The validated extended glucoregulatory model was used for in silico studies. The model replicated a clinical study of the effect of glucagon at varying insulin levels. The simulations also suggested new glucagon doses to be tested in a similar in vivo study to provide new insight to the relationship between insulin, glucagon, and EGP. Finally, the model was used to conduct a large original simulation study investigating an insulin dependent glucagon dosing regimen for treatment of insulin-induced mild hypoglycemia.

General information
State: Published
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With dwindling easily accessible oil and gas resources, more and more exploration and production activities in the oil industry are driven to technically challenging environments such as unconventional resources and deeper formations. The temperature and pressure can become extremely high, e.g., up to 250 °C and 2400 bar, in the deep petroleum reservoirs. Furthermore, many of these deep reservoirs are found offshore, including the North Sea and the Gulf of Mexico, making the development even more risky. On the other hand, development of these high pressure high temperature (HPHT) fields can be highly rewarding if successfully produced. This PhD project is part of the NextOil (New Extreme Oil and Gas in the Danish North Sea) project which is intended to reduce the uncertainties in HPHT field development. The main focus of this PhD is an accurate description of the reservoir fluid behavior under HPHT conditions to minimize the production risks from these types of reservoirs. In particular, the study has thoroughly evaluated several non-Cubic Equations of State (EoSs) which are considered promising for HPHT fluid modeling, showing their advantages and short comings based on an extensive comparison with experimental data. In the course of the evaluation, we have developed new petroleum fluid characterization procedures, built large databases for well-defined mixtures and reservoir fluids, and improved the evaluation software and made it more suitable for efficient and large scale comparison. We have made a comprehensive comparison between cubic and non-cubic EoSs to evaluate whether advanced EoS in non-cubic forms, including both the SAFT-type EoS with strong theoretical basis (e.g. the PC-SAFT EoS) and the empirical BWR-type EoS (e.g. the Soave-BWR EoS), can be advantageous for describing the physical properties and phase equilibrium of reservoir fluids over a wide temperature and pressure range. In addition, we have also compared these models in calculation of heat capacities and Joule-Thomson coefficients for pure components and multicomponent mixtures. Joule-Thomson coefficients are of special interest to the oil industry because of the so called reverse Joule-Thomson effect commonly observed in HPHT fields, where a decrease in pressure results in an increase in temperature, which is just the opposite to the effect at low pressure. In the comparative studies between cubic and non-cubic models, we also included GERG-2008 which is a wide-range EoS developed for 21 components of natural gases and their binary mixtures and is regarded as the most accurate EoS model for natural gas mixtures. It was found that the non-cubic models are much better than the cubics in density, compressibility, heat capacity and Joule-Thomson coefficient calculation of the well defined light and heavy components in reservoir fluids over a wide temperature and pressure range, GERG-2008 being the best with the lowest deviation among all EoS models. GERG-2008 however gives very large deviations for bubble point pressure calculation of some heavy and asymmetric binary systems such as n-butane + n-nonane system. This suggests that this EoS and its binary interaction parameters could still be improved for some of the binary pairs. Soave-BWR gives the closest prediction of the thermal properties to that of GERG-2008 among other EoSs tested in this study. The binary VLE calculation showed that PC-SAFT and Soave-BWR are similar to SRK and PR in correlating the important binary pairs in reservoir fluids. Although Soave-BWR and PC-SAFT give smaller average kij values than SRK and PR, they are more sensitive to the change in kij. Phase envelope prediction of synthetic gases showed that all the EoS models were similar for not too asymmetric synthetic gases, with or without the optimal kij values for SRK, PR, PC-SAFT and Soave-BWR. For highly asymmetric synthetic mixtures, Soave-BWR and GERG-2008 tend to predict phase envelopes different from other models where as none of the tested models give satisfactory predictions. For heat capacity and Joule-Thomson coefficients, GERG-2008 and Soave-BWR give the closest predictions. All the evaluated EoS models tend to predict a nearly constant Joule-Thomson coefficient at high pressures. For typical reservoir temperatures, the constant is around -0.5 K/MPa. For non-cubic models like PC-SAFT the characterization method is less mature than the cubic models. A reservoir fluid characterization method for PC-SAFT has been proposed by combining Pedersen’s method with a newly developed set of correlations for the PC-SAFT model parameters m, m/k and m2. In addition, we further improved the characterization method for PC-SAFT by adjusting the correlations with a large PVT database. We have further improved the correlations and more importantly, we have established a general approach to characterizing reservoir fluids for any EoS. The approach consists in developing correlations of model parameters first with a database for well-defined components and then adjusting the correlations with a large PVT database. The adjustment is made to minimize the deviation in key PVT properties like saturation pressures, densities at reservoir temperature and Stock Tank Oil (STO) densities, while keeping the n-alkane limit of the correlations unchanged. Apart from applying this general approach to PC-SAFT, we have also shown that the approach can be applied to classical cubic models like SRK and PR. In addition, we discussed how to develop a PNA based characterization for PC-SAFT and also utilize a large PVT database to further improve the characterization. With the developed characterization methods, we have made a comparison in PVT calculation involving 17 EoS-characterization combinations and 260 reservoir fluids. PC-SAFT with the new general characterization method is shown to give the lowest AAD% and maximum deviation in calculation of saturation pressure, density and STO density, among all the tested characterization methods for PC-SAFT. Application of the new characterization method to SRK and PR improved the saturation pressure calculation in comparison to the original characterization method for SRK and PR. Using volume translation together with the new characterization approach for SRK and PR gives comparable results for density and STO density to that of original characterization for SRK and PR with volume translation. For the PVT database
used in this study, cubic EoSs seem to have better performance than PC-SAFT in calculation of saturation pressure; PC-SAFT and cubics with volume translation show comparable results in calculation of density and STO density. As a preliminary attempt to integrate more analytical information in characterization, we discussed how to modify the existing algorithms to utilize data from both simulated distillation and true boiling point distillation, and in particular, the component distribution information from the simulated distillation. Some analyses have been made on the impact of including more detailed analytical information. Finally, to improve Soave-BWR for mixture calculation, we have tried to develop several new sets of mixing rules for this EoS. The new mixing rules were developed based on some theoretical considerations as well as the previous mixing rules for non-cubic EoS models. In addition, it was tried to create some hybrid mixing rules by combining a new set of mixing rules and the original mixing rules for Soave-BWR. It was shown that some problems with the original Soave-BWR mixing rules can be fixed by the new mixing rules although the overall performance is not significantly improved. Development of mixing rules for non-cubic EoS models is still a semi-empirical process, requiring extensive testing to evaluating their performance. We have developed the code in a structured manner so that the new mixing rules can be quickly tested. It can facilitate further extensive screening of new mixing rules for Soave-BWR or even other non-cubic EoS models.

General information
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Multilevel techniques for Reservoir Simulation
The subject of this thesis is the development, application and study of novel multilevel methods for the acceleration and improvement of reservoir simulation techniques. The motivation for addressing this topic is a need for more accurate predictions of porous media flow and the ability to carry out these computations in a timely manner. This will lead to better decision making in the production of oil and gas. The goal is attained in various ways throughout the thesis work. Specifically, three fields of multilevel methods have been addressed in this work, namely

•Nonlinear multigrid (the Full Approximation Scheme)
•Variational (Galerkin) upscaling
•Linear solvers and preconditioners

First, a nonlinear multigrid scheme in the form of the Full Approximation Scheme (FAS) is implemented and studied for a 3D three-phase compressible rock/fluids immiscible reservoir simulator with a coupled well model. In a fair way, it is compared to the state-of-the-art solution scheme used in industry and research simulators. It is found that FAS improves time-to-solution by having a larger basin of attraction, faster initial convergence, data locality and a lower memory footprint. The study is extended to include a hybrid strategy, where FAS is combined with Newton’s method to construct a multilevel nonlinear preconditioner. This method demonstrates high efficiency and robustness.

Second, an improved IMPES formulated reservoir simulator is implemented using a novel variational upscaling approach based on element-based Algebraic Multigrid (AMGe). In particular, an advanced AMGe technique with guaranteed approximation properties is used to construct a coarse multilevel hierarchy of Raviart-Thomas and L2 spaces for the Galerkin coarsening of a mixed formulation of the reservoir simulation equations. By experimentation it is found that the AMGe based upsampling technique provided very accurate results while reducing the computational time proportionally to the reduction in degrees of freedom. Furthermore, it is demonstrated that the AMGe coarse spaces (interpolation operators) can be used for both variational upsampling and the construction of linear solvers. In particular, it is found to be beneficial (or even necessary) to apply an AMGe based multigrid solver to solve the upscaled problems. It is found that the AMGe upsampling changes the spectral properties of the matrix, which renders well-known state-of-the-art solvers for this type of system useless.

Third, FAS is combined with AMGe with guaranteed approximation properties to obtain a nonlinear multigrid solver for
unstructured meshes. The FAS-AMGe solver is applied to a simplistic but numerically challenging mixed (velocity-/pressure) model for porous media flow. In a fair way, FAS-AMGe is compared to Newton’s method and Picard iterations. It is found that FAS-AMGe is faster for the cases considered.

Finally, a number of multigrid linear solvers and preconditioners are implemented for various linear systems. In particular AMGe are used in the construction of multigrid preconditioners. These are compared to two state-of-the-art block diagonal preconditioners based on 1) a Schur complement with an Algebraic Multigrid (AMG) solver and 2) an augmented Lagrangian formulation using the Auxiliary Space AMG solver.

In addition to the research mentioned above, a sequential in-house COmpositional reservoir SImulator (COSI) with many features is parallelized in a distributed setting (MPI) using the PETSc framework. A parallel preconditioner based on the Constrained Pressure Residual method, Algebraic Multigrid and Restricted Additive Overlapping Schwarz with Incomplete LU solves on each subdomain is implemented. It is found that switching the traditionally used method, namely parallel ILU, with Restricted Additive Overlapping Schwarz results in a significant increase in parallel scalability while still maintaining similar robustness and efficiency.

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Multiple shooting applied to robust reservoir control optimization including output constraints on coherent risk measures
The production life of oil reservoirs starts under significant uncertainty regarding the actual economical return of the recovery process due to the lack of oil field data. Consequently, investors and operators make management decisions based on a limited and uncertain description of the reservoir. In this work, we propose a new formulation for robust optimization of reservoir well controls. It is inspired by the multiple shooting (MS) method which permits a broad range of parallelization opportunities and output constraint handling. This formulation exploits coherent risk measures, a concept traditionally used in finance, to bound the risk on constraint violation. We propose a reduced sequential quadratic programming (rSQP) algorithm to solve the underlying optimization problem. This algorithm exploits the structure of the coherent risk measures, thus a large set of constraints are solved within sub-problems. Moreover, a variable elimination procedure allows solving the optimization problem in a reduced space and an iterative active-set method helps to handle a large set of inequality constraints. Finally, we demonstrate the application of constraints to bound the risk of water production peaks rather than worst-case satisfaction.

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Numerical Multilevel Upscaling for Incompressible Flow in Reservoir Simulation: An Element-based Algebraic Multigrid (AMGe) Approach

We study the application of a finite element numerical upscaling technique to the incompressible two-phase porous media total velocity formulation. Specifically, an element agglomeration based Algebraic Multigrid (AMGe) technique with improved approximation proper ties [37] is used, for the first time, to generate upscaled and accurate coarse systems for the reservoir simulation equations. The upscaling technique is applied to both the mixed system for velocity and pressure...
and to the hyperbolic transport equations providing fully upscaled systems. By introducing additional degrees of freedom associated with non-planar interfaces between agglomerates, the coarse velocity space has guaranteed approximation properties. The employed AMGe technique provides coarse spaces with desirable local mass conservation and stability properties analogous to the original pair of Raviart-Thomas and piecewise discontinuous polynomial spaces, resulting in strong mass conservation for the upscaled systems. Due to the guaranteed approximation properties and the generic nature of the AMGe method, recursive multilevel upscaling is automatically obtained. Furthermore, this technique works for both structured and unstructured meshes. multiscale Mixed Finite Elements exhibit accuracy for general unstructured meshes but do not in general lead to nested hierarchy of spaces. Multiscale multilevel mimetic finite differences generate nested spaces but lack the adaptivity of the flux representation on coarser levels that the proposed AMGe approach offers. Thus, the proposed approach can be seen as a rigorous bridge that merges the best properties of these two existing methods. The accuracy and stability of the studied multilevel AMGe upscaling technique is demonstrated on two challenging test cases.

General information
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    Scopus rating (2010): SJR 1.65 SNIP 1.768
    BFI (2009): BFI-level 2
    Scopus rating (2009): SJR 2.092 SNIP 1.883
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Offset Risk Minimization for Open-loop Optimal Control of Oil Reservoirs

Simulation studies of oil field water flooding have demonstrated a significant potential of optimal control technology to improve industrial practices. However, real-life applications are challenged by unknown geological factors that make reservoir models highly uncertain. To minimize the associated financial risks, the oil literature has used ensemble-based methods to manipulate the net present value (NPV) distribution by optimizing sample estimated risk measures. In general, such methods successfully reduce overall risk. However, as this paper demonstrates, ensemble-based control strategies may result in individual profit outcomes that perform worse than real-life dominating strategies. This poses significant financial risks to oil companies whose main concern is to avoid unacceptable low profits. To remedy this, this paper proposes offset risk minimization. Unlike existing methodology, the offset method uses the NPV offset distribution to minimize risk relative to a competing reference strategy. Open-loop simulations of a 3D two-phase synthetic reservoir demonstrate the potential of offset risk minimization to significantly improve the worst case profit offset relative to real-life best practices. The results suggest that it may be more relevant to consider the NPV offset distribution than the NPV distribution when minimizing risk in production optimization.

General information
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Permeability in deep North Sea sandstones as predicted from NMR

General information
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Organisations: Department of Civil Engineering, Section for Geotechnics and Geology, Center for Energy Resources Engineering
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Main Research Area: Technical/natural sciences

Phase Equilibrium Modeling for Shale Production Simulation

Production of oil and gas from shale reservoirs has gained more attention in the past few decades due to its increasing economic feasibility and the size of potential sources around the world. Shale reservoirs are characterized by a more tight nature in comparison with conventional reservoirs, having pore size distributions ranging in the nanometer scale. Such a confined nature introduces new challenges in the fluid phase behavior. High capillary forces can be experienced between the liquid and vapor, and selective adsorption of components onto the rock becomes relevant. The impact of these effects is of great importance to understanding the storage of hydrocarbons inside and to forecasting its production. In this thesis, a study focused on the effects of capillary pressure and adsorption on phase behavior, and their impact on oil production is provided. An efficient algorithm for phase envelope calculations in the presence of the capillary pressure is presented, and it is used to analyze the main changes on the phase boundary for several fluids of interest. The results show changes in the saturation pressure and temperature along the phase envelope, except at the critical point. A linear analysis is presented to explain such changes, as a result, useful mathematical relationships that estimate the magnitude of these changes were obtained. Moreover, a flash algorithm that accounts for capillarity was developed. The algorithm was implemented into a fully implicit compositional reservoir simulator, which was then used to assess the impact of the capillary pressure on phase behavior in oil and gas production from tight reservoirs. Since capillary pressure and adsorption occur simultaneously in shale, its combined effect was studied. A model comparison for high-pressure adsorption in shale is presented. The adsorption data in shale is generally scarce, therefore, additional capabilities besides the accuracy were considered in the comparison. The multicomponent potential theory of adsorption yields the best results. Moreover, it shows to be useful to extrapolate adsorption data for hydrocarbons that are not available in the literature. An algorithm for phase split calculations considering both capillary pressure and adsorption was developed. The results show that adsorption and capillary pressure can significantly change the phase behavior. In general, a much shrunk phase envelope with a shifted critical point is obtained for hydrocarbon mixtures. Such behavior is mainly caused by compositional changes in the bulk phase due to selective adsorption of the heavier components onto the rock, while the change in bubble point pressure is mainly due to capillary pressure. This study has developed several robust calculation tools for phase equilibrium in porous media with capillary pressure and adsorption effects. Analysis using these tools have shown that capillary pressure and adsorption have non-negligible effects on phase equilibrium in shale. As general tools, they can be used to calculate phase equilibrium in other porous media as well. The compositional simulator with added capillary pressure effects on phase equilibrium can be used for evaluating the effects in dynamic and more complex scenarios.

General information
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Rock Physics

Rock physics is the discipline linking petrophysical properties as derived from borehole data to surface based geophysical exploration data. It can involve interpretation of both elastic wave propagation and electrical conductivity, but in this chapter focus is on elasticity. Rock physics is based on continuum mechanics, and the theory of elasticity developed for statics becomes the key to petrophysical interpretation of velocity of elastic waves. In practice, rock physics involves interpretation of well logs including vertical seismic profiling (VSP) and analysis of core samples. The results of these procedures are then integrated with reflection seismic data (Japsen, Bruun et al. 2004; Al-Shuhail 2007).

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Rock Properties
Seasonal Deep Aquifer Thermal Energy Storage in the Gassum Sandstone Formation

Seasonal storage of excess heat in hot deep aquifers is considered to optimise the usage of commonly available energy sources. The potential chemical reactions caused by heating the Gassum Sandstone Formation to up to 150°C is investigated by core flooding experiments combined with petrographic analysis and geochemical modelling. Synthetic formation water is injected into two sets of Gassum Formation samples at 25°C, 50°C (reservoir temperature), 100°C and 150°C with a velocity of 0.05 PV/hr and 0.1 PV/hr, respectively. A significant increase in the aqueous concentration of silicium and iron with increasing temperature is observed due to dissolution of silica and siderite. Increasing the reservoir temperature from 50°C to 100°C enhanced the naturally occurring weathering of Na-rich feldspar to kaolinite. Dissolution of quartz increased sharply above 100°C and was the dominating process at 150°C. At temperatures ≤100°C, the silicium concentration was controlled by a dynamic equilibrium between feldspar dissolution and kaolinite precipitation while the concentration was kinetically controlled by quartz dissolution at 150°C. The results imply that storage of excess heat in the Gassum Formation in the Stenlille area may be possible provided operational precautions are taken.

Temperature Effects on Stiffness Moduli of Reservoir Sandstone from the Deep North Sea

We investigate effect of testing temperature on the dynamic frame stiffness of quartz-bearing North Sea sandstone from depths of 5 km. We show that at low stress levels, the rock frame stiffens with increasing temperature and we propose an explanation for the controlling mechanisms. While equilibrating to atmospheric conditions, cooling and stress release of reservoir material can induce tensional forces in the rock frame leading to ruptures of the contact cement in the weakest grain contacts. The frame stiffness hence reduces, as the ruptures are permanent. However, a fraction of the in-situ stiffness can be restored by reestablishment of reservoir stress or temperature, but only as recovery of contact between ruptures and not as re-cementation. In literature, ruptures of contact cement are denoted as micro-cracks, strictly posing a bulk term, without distinguishing effects of stress from temperature. This is unfortunate and hence, we designed a testing program with the intension of separating and quantifying effects of temperature and stress, specifically for the sandstone material subject to this study.
**The Adjoint Method for Gradient-based Dynamic Optimization of UV Flash Processes**

This paper presents a novel single-shooting algorithm for gradient-based solution of optimal control problems with vapor-liquid equilibrium constraints. Dynamic optimization of UV flash processes is relevant in nonlinear model predictive control of distillation columns, certain two-phase flow problems, and oil reservoir production with significant compositional and thermal effects. Gradients are computed with the adjoint method and we use various optimization software (fmincon, IPOPT, KNITRO, and NPSOL) for the numerical optimization. We present computational results for a non-ideal five-component flash process which demonstrate the importance of the optimization solver, the compiler, and the linear algebra software for the efficiency of dynamic optimization of UV flash processes.

**General information**

State: Published
Organisations: Department of Applied Mathematics and Computer Science, Scientific Computing, Center for Energy Resources Engineering
Authors: Ritschel, T. K. S. (Intern), Capolei, A. (Intern), Jørgensen, J. B. (Intern)
Pages: 2071-2076
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**Thermal conductivity of sedimentary rocks as function of Biot's coefficient**

A theoretical model for prediction of effective thermal conductivity with application to sedimentary rocks is presented. Effective thermal conductivity of sedimentary rocks can be estimated from empirical relations or theoretically modelled. Empirical relations are limited to the empirical conditions and should be applied with caution. Theoretical models are typically porosity-based and unable to capture the complexity of sedimentary rocks. We propose a theoretical model, derived from measurable para-meters including both quantity and connectivity of the constituents. Because the thermal conductivity of solids is typically orders of magnitude larger than that of fluids, grain contacts constituting the solid connectivity governs the heat transfer of sedimentary rocks and hence should be the basis for modelling effective thermal conductivity. By introducing Biot's coefficient, $\alpha$, we propose $(1 - \alpha)$ as a measure of the solid connectivity and show how effective thermal conductivity of water saturated and dry sandstones can be modelled.

**General information**

State: Published
Organisations: Department of Civil Engineering, Section for Geotechnics and Geology, Center for Energy Resources Engineering, Technical University of Denmark, German Research Centre for Geosciences
Authors: Orlander, T. (Intern), Pasquinelli, L. (Intern), Asmussen, J. (Ekstern), Marczyński, A. (Ekstern), Adamopoulou, E. (Ekstern), Milsch, H. (Ekstern)
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Main Research Area: Technical/natural sciences
Source: PublicationPreSubmission
Upscaling of enzyme enhanced CO2 capture

Fossil fuels are the backbone of the energy generation in the coming decades for USA, China, India and Europe, hence high greenhouse gas emissions are expected in future. Carbon capture and storage technology (CCS) is the only technology that can mitigate greenhouse gas emissions from fossil fuel fired power by selectively capturing CO2 from flue gases. High capital and high operational costs of this process are the major obstacles of industrial implementation. In the field of CCS the chemical absorption process is the most mature technology. The use of kinetic rate promoters that enhance the mass transfer of CO2 with slow-capturing but energetically favorable solvents can open up a variety of new process options for this technology.

The ubiquitous enzyme carbonic anhydrase (CA), which enhances the mass transfer of CO2 in the lungs by catalyzing the reversible hydration of CO2, is one very promising mass transfer rate promoter for CCS. This process has been previously been tested successfully in lab scale and in some rare cases in pilot scale, but no validated process model for this technology has been published yet.

This PhD thesis presents an investigation of the feasibility of enzyme enhanced CO2 capture technology by identifying the potentials and limitations in lab and in pilot scale and benchmarking the process against proven technologies. The main goal was to derive a realistic process model for technical size absorbers with a wide range of validity incorporating a mechanistic enzyme kinetic model and validating it against in-house pilot plant experiments.

The work consisted of identifying a suitable enzyme-solvent system and the ideal process conditions by comparing mass transfer rates of different solvents and enzyme enhanced solvents in a lab scale wetted wall column. A kinetic model for the mechanistic enzyme reactions was developed for MDEA (Nmethyl-diethanolamine) solutions capable of describing the mass transfer of CO2 for absorption and desorption. It incorporates the influence of all relevant process conditions for technical absorbers, such as: temperature, solvent concentration, enzyme concentration, CO2 concentration in the gas and liquid phase, as well as bicarbonate concentration in the liquid phase.

The process with enzyme enhanced MDEA was scaled up, and absorption experiments were carried out on a 10 m high pilot absorber column. The influence of enzyme concentration, column height, as well as solvent flow rates were determined for 30 wt% MDEA in over 50 runs and compared to over 30 pilot plant runs with the industrial standard solvent 30 wt% MEA (monoethanolamine) under the same process conditions. The mass transfer performance of enzyme enhanced solutions was found to be close to the industrial standard.

The pilot plant experiments could be accurately predicted with the in-house absorber column model CAPCO2 after the kinetic enzyme model from the lab experiments was implemented. The model can very accurately simulate the influence of each process parameter tested.

For targeting the thermal stability of the enzyme in desorption, an alternative low temperature process without reboiler was presented. A stripping gas carrier is utilized in this process to avoid thermal deactivation of the enzymes in the solvent regeneration; its technical feasibility was successfully tested in pilot scale desorption experiments.

The experiments at lab and pilot scale have clearly proven CA’s potential in CCS. The presented validated absorber column model together with the low temperature regeneration process can be used to simulate and optimize the enzyme enhanced CO2 capture process and benchmark this novel technology against conventional processes.
Validation of a Simulation Model Describing the Glucose-Insulin-Glucagon Pharmacodynamics in Patients with Type 1 Diabetes

Currently, no consensus exists on a model describing endogenous glucose production (EGP) as a function of glucagon concentrations. Reliable simulations to determine the glucagon dose preventing or treating hypoglycemia or to tune a dual-hormone artificial pancreas control algorithm need a validated glucoregulatory model including the effect of glucagon.

General information
State: Published
Organisations: Department of Applied Mathematics and Computer Science, Scientific Computing, Dynamical Systems, Copenhagen Center for Health Technology, Center for Energy Resources Engineering, Copenhagen University Hospital, Zealand Pharma A/S, University of Copenhagen
Authors: Wendt, S. L. (Intern), Ranjan, A. (Ekstern), Møller, J. K. (Intern), Schmidt, S. (Ekstern), Boye Knudsen, C. (Ekstern), Holst, J. J. (Ekstern), Madsbad, S. (Ekstern), Madsen, H. (Intern), Nørgaard, K. (Ekstern), Jørgensen, J. B. (Intern)
Number of pages: 1
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Water-Oil Emulsions with Fines in Smart Water Enhanced Oil Recovery

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Organisations: Department of Chemical and Biochemical Engineering, CERE – Center for Energy Ressources Engineering, Center for Energy Resources Engineering
Authors: Arshad, M. W. (Intern), Fosbøl, P. L. (Intern), Shapiro, A. (Intern), Thomsen, K. (Intern)
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Publication: Research - peer-review › Article in proceedings – Annual report year: 2017

Water saturation and stiffness of chalk from Halfdan and Dan fields, Danish North Sea

General information
State: Published
Organisations: Department of Civil Engineering, Section for Geotechnics and Geology, Center for Energy Resources Engineering, Danish Hydrocarbon Research and Technology Centre
Authors: Meireles, L. T. P. (Intern), Welch, M. J. (Ekstern), Fabricius, I. L. (Intern)
A collocation method for surface tension calculations with the density gradient theory

Surface tension calculations are important in many industrial applications and over a wide range of temperatures, pressures and compositions. Empirical parachor methods are not suitable over a wide condition range and the combined use of density gradient theory with equations of state has been proposed in literature. Often, many millions of calculations are required in the gradient theory methods, which is computationally very intensive. In this work, we have developed an algorithm to calculate surface tensions an order of magnitude faster than the existing methods, with no loss of accuracy. The new method can be used with any equation of state, and gives much improved performance. In this work, the new method for solving the gradient density theory equations is combined with cubic equations of state and the Cubic-Plus-Association model. Applications for both binary and multicomponent mixtures and for both hydrocarbon and associating systems are shown. For most systems, the predictions obtained are in good agreement with experimental data. However, cases have been identified where further investigation is needed.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering
Authors: Larsen, P. M. (Intern), Maribo-Mogensen, B. (Intern), Kontogeorgis, G. M. (Intern)
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Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
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Web of Science (2015): Indexed yes
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Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.152 SNIP 1.286 CiteScore 2.31
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.034 SNIP 1.234 CiteScore 2.26
A comment on water’s structure using monomer fraction data and theories

Monomer fraction data for water (and other compounds) can provide useful information about their structure and can be used in “advanced” equations of state, which account explicitly for association phenomena. Recent findings about the performance of association theories in representing the monomer fraction of water are reviewed. Three such theories are considered and all of them perform qualitatively similar. They can all represent phase equilibria for water solutions qualitatively well but with parameters which are not in good agreement with Luck’s famous monomer fraction data. While this could set the theoretical basis of these theories in doubt, we also show in this work that the findings with these association models are in agreement with a recently presented theory which links monomer fraction to dielectric constants. This new theory, like the three thermodynamic models, predicts more hydrogen bonding in water than Luck’s data (Angew. Chem. Int. Ed. Engl. 1980, vol. 19, pp. 28). Moreover, it appears that both the new theory and the three models provide evidence for the four-site association scheme for water and thus support that the tetrahedral structure of the water molecule is correct or at least that the tetrahedral structure is in agreement with several pure water physical properties, monomer fraction information and phase equilibria data in mixtures with alkanes.
A Layout for the Carbon Capture with Aqueous Ammonia without Salt Precipitation

Post-combustion carbon capture technologies seem to be necessary to realize the CO2 mitigation policies internationally shared for the next future, despite none of them appears to be ready for full-scale applications. This work considers the aqueous ammonia based process for a coal-fired Ultra Super Critical power plant. Two layouts are simulated with Aspen Plus employing the recently recalibrated Extended UNIQUAC thermodynamic model. The first one operates at chilling conditions, which yield to salt precipitation, and is taken as reference because already analyzed in previous studies. The second layout operates at cooled conditions, which does not yield any salt precipitation. The Chilled layout reveals low specific heat duty and SPECCA equal to 2.2 and 2.86 MJ/kgco2, respectively. In contrast, the Cooled layout presents a higher specific heat duty of almost 3 MJ/kgco2 but, importantly, a lower SPECCA of 2.58 MJ/kgco2. The latter layout is a better choice also from the perspective of the plant operation since it does not present the salt precipitation.

General information
State: Published
Organisations: Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resouces Engineering, Politecnico di Milano
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BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.425 SNIP 0.785 CiteScore 1.02
ISI indexed (2013): ISI indexed no
Web of Science (2013): Indexed yes
Scopus rating (2012): SJR 0.425 SNIP 0.563 CiteScore 1.08
ISI indexed (2012): ISI indexed no
Web of Science (2012): Indexed yes
Scopus rating (2011): SJR 0.918 SNIP 1.505 CiteScore 2.42
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Original language: English
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A_Layout_for_the_Carbon_Capture_with_Aqueous_Ammonia_without_Salt_Precipitation.pdf
Algorithms and Methods for High-Performance Model Predictive Control

The goal of this thesis is to investigate algorithms and methods to reduce the solution time of solvers for Model Predictive Control (MPC). The thesis is accompanied with an open-source toolbox for High-Performance implementation of solvers for MPC (HPMPC), that contains the source code of all routines employed in the numerical tests. The main focus of this thesis is on linear MPC problems.

In this thesis, both the algorithms and their implementation are equally important. About the implementation, a novel implementation strategy for the dense linear algebra routines in embedded optimization is proposed, aiming at improving the computational performance in case of small matrices. About the algorithms, they are built on top of the proposed linear algebra, and they are tailored to exploit the high-level structure of the MPC problems, with special care on reducing the computational complexity.

An open-source thermodynamic software library

This is a technical report which accompanies the article "An open-source thermodynamic software library" which describes an efficient Matlab and C implementation for evaluation of thermodynamic properties. In this technical report we present the model equations, that are also presented in the paper, together with a full set of first and second order derivatives with respect to temperature and pressure, and in cases where applicable, also with respect to mole numbers. The library is based on parameters and correlations from the DIPPR database and the Peng-Robinson and the Soave-Redlich-Kwong equations of state.
Block-sparse beamforming for spatially extended sources in a Bayesian formulation

Direction-of-arrival (DOA) estimation refers to the localization of sound sources on an angular grid from noisy measurements of the associated wavefield with an array of sensors. For accurate localization, the number of angular directions is much larger than the number of sensors, hence, the problem is underdetermined and requires regularization. Traditional methods use an L2-norm regularizer, which promotes minimum-power (smooth) solutions, while regularizing with L1-norm promotes sparsity. Sparse signal reconstruction improves the resolution in DOA estimation in the presence of a few point sources, but cannot capture spatially extended sources. The DOA estimation problem is formulated in a Bayesian framework where regularization is imposed through prior information on the source spatial distribution which is then reconstructed as the maximum a posteriori estimate. A composite prior is introduced, which simultaneously promotes a piecewise constant profile and sparsity in the solution. Simulations and experimental measurements show that this choice of regularization provides high-resolution DOA estimation in a general framework, i.e., in the presence of spatially extended sources.

General information
State: Published
Organisations: Center for Energy Resources Engineering, Department of Applied Mathematics and Computer Science, National Space Institute, Department of Informatics and Mathematical Modeling, Department of Electrical Engineering, Acoustic Technology, University of California, San Diego
Authors: Xenaki, A. (Intern), Fernandez Grande, E. (Intern), Gerstoft, P. (Ekstern)
Pages: 1828-1838
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Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 0.788 SNIP 1.423 CiteScore 1.8
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 0.705 SNIP 1.966 CiteScore 2
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Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 0.763 SNIP 1.622 CiteScore 1.75
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 0.695 SNIP 1.642 CiteScore 1.68
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 0.754 SNIP 1.528
Web of Science (2010): Indexed yes
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Scopus rating (2008): SJR 0.848 SNIP 1.633
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Web of Science (2007): Indexed yes
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Scopus rating (2003): SJR 0.882 SNIP 1.712
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Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 0.719 SNIP 1.467
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Web of Science (2000): Indexed yes
Scopus rating (1999): SJR 0.591 SNIP 1.319

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Boring og effekter af frakturering

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Authors: Fabricius, I. L. (Intern)
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Controllability and flexibility analysis of CO2 post-combustion capture using piperazine and MEA

In this study, we developed a decentralized control scheme and investigate the performance of the piperazine (PZ) and monoethanolamine (MEA) CO2 capture process for industrially-relevant operation scenarios. The base for the design of the control schemes is Relative Gain Array (RGA) analysis combined with open-loop dynamic sensitivity analysis.

This study suggests that controllers with smaller time integrals and larger gains are required to maintain the PZ plant within reasonable short closed-loop settling times when compared to MEA. It also shows that the offset from the designated set-points in the presence of disturbances in the flue gas flow and heat duty is larger using PZ compared to MEA. The settling time for the PZ plant is generally larger than for MEA. However, the PZ plant rejects the disturbances faster and with less variability in the load of the power plant. Furthermore, this study indicates that the proposed PI-based control structure can handle large changes in the load provided that the manipulated variables, i.e. lean solvent flow or reboiler duty, do not reach their saturation limit. Additionally, we observed that shortage in the steam supply (reboiler duty) may represent a critical operational bottleneck, especially when PZ is being used. The MEA plant controllers drive the system towards drying out/flooding while the CO2 capture rate performance of the PZ plant reduces drastically in the presence of constraints in the availability of steam. These findings suggest the need for advanced control structures, e.g. MPC, which can explicitly account for constraints in the process variables.

General information
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Organisations: Center for Energy Resources Engineering, Department of Applied Mathematics and Computer Science, Scientific Computing, CERE – Center for Energy Ressources Engineering, Copenhagen Center for Health Technology, Department of Chemical and Biochemical Engineering, University of Waterloo
Authors: Gaspar, J. (Intern), Ricardez-Sandoval, L. (Ekstern), Jørgensen, J. B. (Intern), Fosbøl, P. L. (Intern)
Pages: 276-289
Publication date: 2016
Main Research Area: Technical/natural sciences
Determining optimum aging time using novel core flooding equipment

New methods for enhanced oil recovery are typically developed using core flooding techniques. Establishing reservoir conditions is essential before the experimental campaign commences. The realistic oil-rock wettability can be obtained through optimum aging of the core. Aging time is affected by temperature, crude oil, formation brine, and coreplug lithology. Minimum time can significantly reduce the experimental cost while insufficient aging time can result in false conclusions. Real-time online resistivity measurements of coreplugs are presented and a novel method is introduced for determining the optimum aging time regardless of variations in crude oil, rock, and brine properties. State of the art core flooding equipment has been developed that can be used for consistently determining the resistivity of the coreplug during aging and waterflooding using advanced data acquisition software. In the proposed equipment, independent axial and sleeve pressure can be applied to mimic stresses at reservoir conditions. 10 coreplugs (four sandstones and six chalk samples) from the North Sea have been aged for more than 408 days in total and more than 29000 resistivity data points have been measured to consistently investigate the change of wettability during aging. At 60°C and 100 bars a homogeneous sandstone coreplug attained optimized wettability after 5 days, a heterogeneous coreplug required 30 days of aging. Chalk coreplugs needed 45 days of aging. This shows that coreplugs originating from the same field, when aged at equivalent conditions can have significantly different aging times because of minor variations in the coreplug properties. No fixed aging time can be recommended on the other hand a method is recommended which can determine the extent of aging. Coreplug aging patterns were studied for variation in pressure (20 to 130 bar) and temperature (60 to 130°C).

General information

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Organisations: Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Ressources Engineering
Distributed Model Predictive Control for Smart Energy Systems

Integration of a large number of flexible consumers in a smart grid requires a scalable power balancing strategy. We formulate the control problem as an optimization problem to be solved repeatedly by the aggregator in a model predictive control framework. To solve the large-scale control problem in real-time requires decomposition methods. We propose a decomposition method based on Douglas–Rachford splitting to solve this large-scale control problem. The method decomposes the problem into smaller subproblems that can be solved in parallel, e.g., locally by each unit connected to an aggregator. The total power consumption is controlled through a negotiation procedure between all cooperating units and an aggregator that coordinates the overall objective. For large-scale systems, this method is faster than solving the original problem and can be distributed to include an arbitrary number of units. We show how different aggregator objectives are implemented and provide simulations of the controller including the computational performance.
Dynamic Operation and Simulation of Post-Combustion CO2 Capture

Thermal power need to operate, on a daily basis, with frequent and fast load changes to balance the large variations of intermittent energy sources, such as wind and solar energy. To make the integration of carbon capture to power plants economically and technically feasible, the carbon capture process has to be able to follow these fast and large load changes without decreasing the overall performance of the carbon capture plant. Therefore, dynamic models for simulation, optimization and control system design are essential. In this work, we compare the transient behavior of the model against dynamic pilot data for CO2 absorption and desorption for step-changes in the flue gas flow rate. In addition we investigate the dynamic behavior of a full-scale post-combustion capture plant using monoethanolamine (MEA) and piperazine (PZ). This analysis demonstrates the good agreement between the developed model (dCAPCO2) and the pilot measurements at both, transient and steady-state conditions. It outlines how the time needed to reach a new steady-state varies with respect to amine type and concentration. The simulation study reveals that it is essential to control the lean solvent flow to avoid sudden changes in the CO2 removal rate and to avoid increased heat demand of solvent regeneration. In addition, it shows how storage tanks (liquid hold-up of the system) can be designed to accommodate significant upstream changes in the power plant management. This flexibility is especially needed for operation in future mixed green energy market. [All rights reserved Elsevier].
General Approach to Characterize Reservoir Fluids Using a Large PVT Database

Global increase in oil demand has resulted in the need for exploring remote and harsh locations where a considerable portion of them are at extreme reservoir temperatures and pressures. Accurate calculation of properties of gas and oil at high pressures and high temperatures (HPHT) is a more prominent issue. Non-cubic Equation of State (EoS) models are an attractive option due to their better description of density and compressibility over a wide temperature and pressure range. Application of these models to reservoir fluids requires development of the corresponding fluid characterization methods. We proposed a general approach to develop correlations for model parameters and applied it to the characterization for the PC-SAFT EoS. The approach consists in first developing the correlations based on the DIPPR database, and then adjusting the correlations based on a large PVT database. The adjustment was made to minimize the deviation in key PVT properties like saturation pressures, densities at reservoir temperature and Stock Tank Oil (STO) densities, while keeping the n-alkane limit of the correlations unchanged. As an improvement of a previously suggested characterization method, the approach gives better PVT calculation results for the tested systems. Comparison was also made between PC-SAFT with the proposed characterization method and other EoS models. The proposed approach can be applied to other EoS models for improving their fluid characterization. Besides, the challenges with PNA based characterization methods are discussed.
kyr. The sparsity of modern-standard data questions the validity (and age range) of this potential geomagnetic asymmetry. In 2013 and 2014, we sampled basaltic lava flows in Jökuldalur, north-eastern Iceland, to obtain high-standard paleodirectional and paleointensity data at relatively high-northern latitudes (65.2°N). On average, we sampled >15 cores per site at 51 sites of predominantly Matuyama age. Complete demagnetization was carried out on all samples using AF or thermal demagnetization. We present 45 distinct paleomagnetic directions based on overall N>10 ChRM per site and α95<3.5°. We obtain a mean direction of \(D=355.7°, I=76.3°\), and \(α95=3.2\) for N=45 sites that is not significantly different from a GAD field. The resulting 45 VGPs distribute around the North Pole, and the global mean paleomagnetic pole \(λ=87.8°, ϕ=224.3°\) is coincident with the North Pole within the α95 confidence limit. We calculate a VGP dispersion \(S_B=4.88\) and an average inclination anomaly \(ΔI=-0.91°\) for our 38 Matuyama age data. The dispersion \(S_B\) overall supports the interpretation of a dependence of \(S_{SB}\) on latitude during the Matuyama, while the negligible \(ΔI\) suggests little deviation from a GAD field. Based on relatively strict cut-off criteria we also present six new field strength estimates from the time interval ∼1.2–1.8 Ma, thus filling a large data gap of the high-northern stable field behavior. We obtain a median VADM of 57±3 ZAm⁻² (VDM of 60±5 Am²), which is higher than the median VADM of 16 intensity estimates from Antarctica (39±7 ZAm⁻²) from the same period. A higher northern field is also found when using less strict cut-off criteria resulting in 14 field estimates from Jökuldalur, i.e. we find support for higher field strength in the northern hemisphere as compared to the southern hemisphere during the Matuyama. Finally, we deliver a revised magneto-chronostratigraphic model of Jökuldalur and conduct an investigation of the type sections of the so-called Gilsá normal polarity event around 1.62 Ma. Our revised model is based on 11 new \(^{40}Ar^{39}Ar\) ages. No evidence is found of the existence of the Gilsá event in Jökuldalur. Instead we find that the normal polarity intervals in the type sections can both be correlated to Olduvai subchron.

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Hydrate Equilibrium Data for CO2+N-2 System in the Presence of Tetra-n-butylammonium Fluoride (TBAF) and Mixture of TBAF and Cyclopentane (CP)

Hydrates can be used for CO2 capture from flue gases (hydrate crystallization). In this work, hydrate equilibrium data were measured and compared with literature data. The isochoric method was used to determine the gas hydrate dissociation points. Different CO2+N2 gas mixtures were used in the presence of promoters such as tetra-n-butylammonium fluoride (TBAF) and mixtures of TBAF and cyclopentane (CP). The key novel aspect of this work is the use of a combination of promoters, TBAF and CP, which under certain conditions induced further pressure reduction in comparison to pure TBAF results. Concerning experiments with pure promoter, there is good agreement between our results and literature results for different gas mixtures and promoter concentrations.

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Hydrate equilibrium data for the CO$_2$ + N$_2$ system with the use of tetra-n-butylammonium bromide (TBAB), cyclopentane (CP) and their mixture
Carbon Dioxide capture and sequestration (CCS) is nowadays an important area of research for decreasing CO₂ emissions worldwide. Hydrates can become of great importance in the future as they form the basis for a new technology that can be used for CO₂ capture from flue gases (hydrate crystallization). In this work hydrate equilibrium data are measured and compared with literature data. In particular, experimental results for hydrate dissociation with several promoters are presented. The isochoric method is used to determine the gas hydrate dissociation points. Different CO₂ + N₂ gas mixtures were used with presence of promoters such as tetra-n-butylammonium bromide (TBAB), cyclopentane (CP) and mixtures of TBAB with CP. The novelty of this work is the combination of promoters, TBAB and CP, which under certain conditions induced greater pressure reduction in comparison to pure TBAB results. Concerning experiments with pure promoters, there is excellent consistency between our results and literature results for different gas mixtures and promoter concentrations. Finally, experimental uncertainties for temperature, pressure, and molar composition are also presented.
Investigation of the Gas Injection Effect on Asphaltene Onset Precipitation Using the Cubic-Plus-Association Equation of State

Miscible and immiscible gas flooding is one of the enhanced oil recovery (EOR) techniques that has been widely used to increase the oil production. One of the critical problems with gas flooding is that it generally aggravates the asphaltene precipitation, which further creates a flow assurance problem. Therefore, it is imperative to investigate beforehand the effect of gas injection into the reservoir from the modeling results. The cubic-plus-association (CPA) equation of state (EoS) has previously been applied to model the asphaltene onset precipitation condition. In this work, we adopt the modeling approach from the previous work and provide the conceptual base for it. Five different reservoir fluids are studied to validate whether the model is able to calculate the effect of different types (e.g., N2, CO2, and methane) and
amounts (e.g., 10, 20, and 30 mol %) of gas injections in agreement with experimental data from the literature. We also investigate the model behavior to show the importance of the association term in the EoS for the selected modeling approach. Sensitivity of the model results when we calculate either two or three model parameters from the experimental data is also studied. Model dependency upon the saturates, aromatics, resins, and asphaltenes (SARA) analysis or molecular weight (MW) of asphaltene is also analyzed. In addition, a unique characteristic of the model for the given stock tank oil (STO) is identified, which does not change with different types and amounts of gas injections and also remains the same at upper and lower onset pressure boundaries. On the basis of this unique characteristic, a simple procedure to predict asphaltene phase envelope (APE) for the reservoir oil with relatively simple and few experimental data, performed on STO with n-pentane/n-heptane as a precipitant, is proposed. This proposed procedure avoids the need of high-pressure measurements of upper onset pressure (UOP).

**General information**

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Irreversible Change of the Pore Structure of ZIF-8 in Carbon Dioxide Capture with Water Coexistence

The performance of zeolitic imidazolate framework 8 (ZIF-8) for CO2 capture under three different conditions (wetted ZIF-8, ZIF-8/water slurry, and ZIF-8/water-glycol slurry) was systemically investigated. This investigation included the study of the pore structure stability of ZIF-8 by using X-ray diffraction, scanning electron microscopy, Fourier transform infrared spectroscopy, and Raman detection technologies. Our results show that the CO2 adsorption ability of ZIF-8 could be substantially increased under the existence of liquid water. However, the structure characterization of the recovered ZIF-8 showed an irreversible change of its framework, which occurs during the CO2 capture process. It was found that there is an irreversible chemical reaction among ZIF-8, water, and CO2, which creates both zinc carbonate (or zinc carbonate hydroxides) and single 2-methylimidazole crystals, and therefore the pore structure of ZIF-8 collapses. It is suggested therefore that care must be taken when using ZIF-8 or products containing ZIF-8 for gas capture, gas separation, or other applications where both water and acid gases coexist.

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Methods and Algorithms for Economic MPC in Power Production Planning

This thesis concerns methods and algorithms for power production planning in contemporary and future power systems. Power production planning is a task that involves decisions across different time scales and planning horizons. Hours-ahead to days-ahead planning is handled by solving a mixed-integer linear program for unit commitment and economic dispatch of the system power generators. We focus on a minutes-ahead planning horizon, where unit commitment decisions are fixed. Economic model predictive control (EMPC) is employed to determine an optimal dispatch for a portfolio of power generators in real-time. A generator can represent a producer of electricity, a consumer of electricity, or possibly both. Examples of generators are heat pumps, electric vehicles, wind turbines, virtual power plants, solar cells, and conventional fuel-fired thermal power plants. Although this thesis is mainly concerned with EMPC for minutes-ahead production planning, we show that the proposed EMPC scheme can be extended to days-ahead planning (including unit commitment) as well.

The power generation from renewable energy sources such as wind and solar power is inherently uncertain and variable. A portfolio with a high penetration of renewable energy is therefore a stochastic system. To accommodate the need for EMPC of stochastic systems, we generalize certainty-equivalent EMPC (CEEMPC) to mean-variance EMPC (MV-EMPC). In MV-EMPC, the objective function is a trade-off between the expected cost and the cost variance. Simulations show that MV-EMPC reduces cost and risk compared to CE-EMPC. The simulations also show that the economic performance of CE-EMPC can be much improved using a constraint back-off heuristic.

Efficient solution of the optimal control problems (OCPs) that arise in EMPC is important, as the OCPs are solved online. We present special-purpose algorithms for EMPC of linear systems that exploit the high degree of structure in the OCPs. A Riccati-based homogeneous and self-dual interior-point method is developed for the special case, where the OCP objective function is a linear function. We design an algorithm based on the alternating direction method of multipliers (ADMM) to solve input-constrained OCPs with convex objective functions. The OCPs that occur in EMPC of dynamically decoupled subsystems, e.g. power generators, have a block-angular structure. Subsystem decomposition algorithms based on ADMM and Dantzig-Wolfe decomposition are proposed to solve these OCPs. Subproblems that arise in the decomposition algorithms are solved using structure-exploiting algorithms. To reduce computation time of the EMPC algorithms further, warm-start and early-termination strategies are employed. Benchmarks show that the special-purpose
algorithms are significantly faster than current state-of-the-art solvers.

As a potential application area of EMPC, we study power production planning in small isolated power systems. A critical part of power production planning in small isolated power systems is operational reserve planning. The operational reserves are activated to balance production and consumption in real-time. An EMPC scheme is presented for activation of operational reserves. Simulations based on a Faroe Islands case study show that significant cost savings can be achieved using this strategy. For efficient planning of the operational reserves, we present an optimal reserve planning problem (ORPP). The ORPP is a contingency-constrained unit commitment problem that addresses low inertia challenges in small isolated power systems.

In summary, the main contributions of this thesis are:
- A mean-variance optimization strategy for EMPC of linear stochastic systems.
- Tailored algorithms for solution of the OCPs that arise in EMPC of linear stochastic systems.
- Methods for power production planning in small isolated power; the ORPP for unit commitment and economic dispatch, and an EMPC scheme for activation of operational reserves.

Modeling and Prediction Using Stochastic Differential Equations

Pharmacokinetic/pharmacodynamic (PK/PD) modeling for a single subject is most often performed using nonlinear models based on deterministic ordinary differential equations (ODEs), and the variation between subjects in a population of subjects is described using a population (mixed effects) setup that describes the variation between subjects. The ODE setup implies that the variation for a single subject is described by a single parameter (or vector), namely the variance (covariance) of the residuals. Furthermore the prediction of the states is given as the solution to the ODEs and hence assumed deterministic and can predict the future perfectly. A more realistic approach would be to allow for randomness in the model due to e.g., the model be too simple or errors in input. We describe a modeling and prediction setup which better reflects reality and suggests stochastic differential equations (SDEs) for modeling and forecasting. It is argued that this gives models and predictions which better reflect reality. The SDE approach also offers a more adequate framework for modeling and a number of efficient tools for model building. A software package (CTSM-R) for SDE-based modeling is briefly described.
Modeling derivative properties and binary mixtures with CO₂ using the CPA and the quadrupolar CPA equations of state

The cubic plus association (CPA) equation of state (EoS) is extended to include quadrupolar interactions. The quadrupolar term is based on a modification of the perturbation terms by Larsen et al. (1977) [5] for a hard sphere fluid with a symmetric point quadrupole moment. The new quadrupolar CPA (qCPA) can be used without introducing any additional pure compound parameters. Alternatively a single additional adjustable parameter can be employed. To evaluate qCPA several pure compound properties are predicted. The model is furthermore evaluated for its ability to predict and correlate binary vapor-liquid equilibria (VLE) and liquid-liquid equilibria (LLE) of mixtures containing CO₂ and hydrocarbons, water, alcohols, or selected quadrupolar compounds. The results indicate that most pure compound property predictions are satisfactory but similar to other CPA approaches. When binary mixtures are considered, qCPA appear to offer a systematic improvement as compared to the cases where quadrupolar interactions are ignored. This improvement is particularly pronounced when mixtures of CO₂ and hydrocarbons are considered, where the model is almost fully predictive. Using the same modeling approach qCPA can accurately correlate both the phase behaviour of CO₂ + hydrocarbon mixtures as well as mixtures of CO₂+a self-associating compound.

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Modeling of phase equilibrium of North Sea oils with water and MEG

The complex phase equilibrium between reservoir fluids and associating compounds like water and glycols has become very important as the increasing global energy demand pushes the oil industry to use advanced methods to increase oil recovery, such as increasing the use of various chemicals to ensure a constant and safe production. The CPA equation of state has been successfully applied in the past to well defined systems and gas condensates containing associating compounds. It has also been extended to reservoir fluids in presence of water and polar chemicals using modified correlations for critical temperature, pressure and acentric factor. In this work, we evaluate CPA using recently developed correlations for predicting the binary interaction parameters between MEG/hydrocarbons and water/hydrocarbons, for a wide range of systems containing reservoir fluids and production chemicals, such as water and ethylene glycol (MEG).

Using these new correlations for prediction of all binary interactions, the CPA EoS satisfactorily describes the mutual solubility of the “binary systems” reservoir fluid and MEG and promising results are also obtained with CPA for ternary mixtures (reservoir fluid + water + MEG), with some deviations for the solubility of hydrocarbons in the polar phase. Improved predictions are observed, when using correlations for binary interactions compared to previous methods of using an average $k_{ij}$ fitted to binary data.

General information
Modelling phase equilibria for acid gas mixtures using the CPA equation of state. Part VI. Multicomponent mixtures with glycols relevant to oil and gas and to liquid or supercritical CO₂ transport applications

In this work the Cubic Plus Association (CPA) equation of state is applied to multicomponent mixtures containing CO₂ with alkanes, water, and glycols. Various modelling approaches are used i.e. different association schemes for pure CO₂ (assuming that it is a non-associating compound, or that it is a self-associating fluid with two, three or four association sites) and different possibilities for modelling mixtures of CO₂ with other hydrogen bonding fluids (only use of one interaction parameter kij or assuming cross association interactions and obtaining the relevant parameters either via a combining rule or using an experimental value for the cross association energy). Initially, new binary interaction parameters were estimated for (CO₂ + glycol) binary mixtures. Having the binary parameters from the binary systems, the model was applied in a predictive way (i.e. no parameters were adjusted to data on ternary and multicomponent mixtures) to model the phase behaviour of ternary and quaternary systems with CO₂ and glycols. It is concluded that CPA performs satisfactorily for most multicomponent systems considered. Some differences between the various modelling approaches are observed. This work is the last part of a series of studies, which aim to arrive in a single "engineering approach" for applying CPA to acid gas mixtures, without introducing significant changes to the model. An overall assessment, based also on the obtained results of this series (Tsivintzelis et al., 2010, 2011, 2014, 2015, 2015), which is based on an investigation of about 30 multicomponent systems containing acid gases, water, alcohols, glycols and hydrocarbons, reveals that assuming cross association (solvation) of CO₂ with glycols, alcohols and water or alternatively considering CO₂ to be a self-associating molecule (with three or four sites) are the better approaches which perform similarly and quite satisfactorily. However, the use of the former one (solvation), using whenever possible experimental values for the cross association energy, in all cases is recommended.
Modelling the glucose-insulin-glucagon dynamics after subcutaneous administration of native glucagon and a novel glucagon analogue in dogs

Zealand Pharma has invented a glucagon analogue, ZP-GA-1, with increased stability in liquid formulation for treatment of hypoglycemia. A pharmacodynamic (PD) model is needed to compare ZP-GA-1 with marketed glucagon. We aim to develop a model of the complex glucose-insulin-glucagon dynamics based on physiology and data.

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Modelling the glucose-insulin-glucagon dynamics after subcutaneous administration of native glucagon and a novel glucagon analogue in dogs

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Model of the Glucose-Insulin-Glucagon Dynamics after Subcutaneous Administration of a Glucagon Rescue Bolus in Healthy Humans

In healthy individuals, insulin and glucagon work in a complex fashion to maintain blood glucose levels within a narrow range. This regulation is distorted in patients with diabetes. The hepatic glucose response due to an elevated glucagon level depends on the current insulin concentration and thus endogenous glucose production (EGP) can not be modelled without knowledge of the concentration of both hormones in plasma. Furthermore, literature suggests an upper limit to EGP irrespective of glucagon levels. We build a simulation model of the glucose-insulin-glucagon dynamics in man including saturation effect of EGP.

Ten healthy subjects received a 1 mg subcutaneous (SC) glucagon bolus (GlucaGen®). Plasma samples were collected until 300 minutes post dose and analyzed for glucagon, insulin, and glucose concentrations. All observations were used to fit a physiological model of the glucose-insulin-glucagon dynamics using the Hovorka model with a novel multiplicative description of the effects of insulin and of glucagon on EGP.

Bayesian estimation by Maximum a Posteriori using prior knowledge reported in literature was used to estimate the model parameters for each subject. Profile likelihood plots were used to investigate parameter identifiability. Unidentifiable parameters were fixed at their prior mean values.

The new model enables simulations of the glucose-insulin-glucagon dynamics in humans at both low and high glucagon concentrations (180-8000 pg/mL) and physiologic insulin concentrations (1.2-81.9 mIU/L). The model can be used for simulation of glucagon bolus strategies for treatment of hypoglycemia and for in silico simulation of dual-hormone artificial pancreas algorithms.
Model of the Glucose-Insulin-Glucagon Dynamics after Subcutaneous Administration of a Glucagon Rescue Bolus in Healthy Humans

In healthy individuals, insulin and glucagon work in a complex fashion to maintain blood glucose levels within a narrow range. This regulation is distorted in patients with diabetes. The hepatic glucose response due to an elevated glucagon level depends on the current insulin concentration and thus endogenous glucose production (EGP) can not be modelled without knowledge of the concentration of both hormones in plasma. Furthermore, literature suggests an upper limit to EGP irrespective of glucagon levels. We build a simulation model of the glucose-insulin-glucagon dynamics in man including saturation effect of EGP.

Ten healthy subjects received a 1 mg subcutaneous (SC) glucagon bolus (GlucaGen®). Plasma samples were collected until 300 minutes post dose and analyzed for glucagon, insulin, and glucose concentrations. All observations were used to fit a physiological model of the glucose-insulin-glucagon dynamics using the Hovorka model with a novel multiplicative description of the effects of insulin and of glucagon on EGP.

Bayesian estimation by Maximum a Posteriori using prior knowledge reported in literature was used to estimate the model parameters for each subject. Profile likelihood plots were used to investigate parameter identifiability. Unidentifiable parameters were fixed at their prior mean values.

The new model enables simulations of the glucose-insulin-glucagon dynamics in humans at both low and high glucagon concentrations (180-8000 pg/mL) and physiologic insulin concentrations (1.2-81.9 mIU/L). The model can be used for simulation of glucagon bolus strategies for treatment of hypoglycemia and for in silico simulation of dual-hormone artificial pancreas algorithms.

Multivariable Optimization of the Piperazine CO2 Post-Combustion Process

8 molal piperazine (PZ) is a promising solvent for developing an energy efficient CO2 post-combustion capture process. However, it has a limited operating range due to precipitation. The operating range can be extended by decreasing the piperazine concentration and/or increasing the CO2 loading of the lean solvent. However, optimal solvent composition must be determined taking into account the solvent circulation rate and the heat demand of the solvent regeneration. In this paper, we determine and generalize trends of performance for a broad range of operating conditions: 1.8 to 9mol PZ/kg water, 0.2 to 0.6 lean loading, and for two flue gas sources: natural gas combined cycle power plant (NGCC, 3.9 mol% CO2).
and a coal based power plant (ASC, 13.25 mol% CO2). Special attention is given to the boundaries where precipitation may occur. The results are created by the hybrid CAPCO2 rate-based model which accounts for precipitation when estimating the heat and mass transfer rates. The results show that the 7 molal piperazine gives the lowest specific reboiler duty at 0.40 CO2 lean loading: 3.32 GJ/t CO2 and 4.05 GJ/t CO2 for the ASC case and NGCC cases. The analysis also reveals that the capture process needs to be operated up to 7.8% above the minimum duty to avoid the risk of clogging due to solid formation. Note, this analysis assumes a 25°C minimum solvent temperature. The energy requirement of the capture process can be further improved by assuming a minimum solvent temperature of 30°C which gives a specific reboiler duty of 3.23 GJ/t CO2 (ASC case) and 3.80 GJ/t CO2 (NGCC case).

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PK/PD modelling of glucose-insulin-glucagon dynamics in healthy dogs after a subcutaneous bolus administration of native glucagon or a novel glucagon analogue

Objective We aim to develop a simulation model of the complex glucose-insulin-glucagon dynamics based on physiology and data. Furthermore, we compare pharmacokinetic (PK) and pharmacodynamic (PD) characteristics of marketed reconstituted glucagon with a stable liquid glucagon analogue invented by Zealand Pharma A/S.

Research Design and Methods We expanded a physiological model of endogenous glucose production with multiplicative effects of insulin and glucagon and combined it with the Hovorka glucoregulatory model. We used a Bayesian framework to perform multidimensional MAP estimation of model parameters given priors reported in the literature. We used profile likelihood analysis to investigate parameter identifiability and reduce the number of model variables. We estimated model parameters in pre-clinical data from one cross-over study with a total of 20 experiments in five dogs. The dogs received two subcutaneous (SC) bolus injections of low and high doses of glucagon and ZP-GA-1 (20 and 120 nmol/kg).

Results We report posterior probability distributions and correlations for all identifiable model parameters. Based on visual inspection and residual analysis, the PD model described data satisfactorily for both glucagon and the analogue. Parameter estimates of the PD model were not significantly different between the two compounds.

Conclusions The new PK/PD model enables simulations of the glucose-insulin-glucagon dynamics after a SC bolus of glucagon or glucagon analogue. The novel glucagon analogue by Zealand Pharma A/S shows PK and PD characteristics similar to marketed glucagon.

General information
State: Published
Organisations: Department of Applied Mathematics and Computer Science, Scientific Computing, Dynamical Systems, Copenhagen Center for Health Technology, Center for Energy Resources Engineering, Zealand Pharma A/S, McGill University
Authors: Wendt, S. L. (Intern), Møller, J. K. (Intern), Boye Knudsen, C. (Ekstern), Madsen, H. (Intern), Haidar, A. (Ekstern), Jørgensen, J. B. (Intern)
Number of pages: 54
Publication date: 2016

Prediction Methods for Blood Glucose Concentration: Design, Use and Evaluation
Standard diabetes insulin therapy for type 1 diabetes and late stages of type 2 is based on the expected development of blood glucose (BG) both as a consequence of the metabolic glucose consumption as well as of meals and exogenous insulin intake. Traditionally, this is not done explicitly, but the insulin amount is chosen using factors that account for this expectation.

The increasing availability of more accurate continuous blood glucose measurement (CGM) systems is attracting much interest to the possibilities of explicit prediction of future BG values. Against this background, in 2014 a two-day workshop on the design, use and evaluation of prediction methods for blood glucose concentration was held at the Johannes Kepler University Linz, Austria. One intention of the workshop was to bring together experts working in various fields on the same topic, in order to shed light from different angles on the underlying problem of modeling the glucose insulin dynamics of type 1 diabetes patients. Among the international participants were continuous glucose monitoring developers, diabetologists, mathematicians and control engineers, both, from academia and industry. In total 18 talks were given followed by panel discussions which allowed to receive direct feedback from the point of view of different disciplines.

This book is based on the contributions of that workshop and is intended to convey an overview of the different aspects involved in the prediction. The individual chapters are based on the presentations given by the authors at the workshop.
but were written afterward which allowed to include the findings and conclusions of the various discussions and of course updates.

The chapter “Alternative Frameworks for Personalized Insulin-Glucose Models” by Harald Kirchsteiger et al. asks the question whether more and more detailed physiological descriptions of the glucose metabolism with an ever-increasing degree of sophistication and number of modeled phenomena are really what is needed for pushing the boundaries in glucose prediction for control. As an alternative, the chapter introduces two data-based approaches that focus not on the prediction of exact future blood glucose values, but rather on the prediction of changes in the patients’ blood glucose range.

The chapter “Accuracy of BG Meters and CGM Systems: Possible Influence Factors for the Glucose Prediction Based on Tissue Glucose Concentrations” by Guido Freckmann et al. discusses performance metrics used to characterize the accuracy of continuous glucose measurement devices. This topic is highly relevant for prediction models since many of them rely on the data given by the continuous sensors which are previously calibrated with blood glucose meter measurements which are also subject to measurement errors. Inaccurate measurements will directly affect the performance of the corresponding predictions.

The chapter “CGM — How Good Is Good Enough?” by Michael Schoemaker and Christopher G. Parkin also tackles the problem of continuous glucose monitor performance evaluation. Several performance metrics used in different published studies are compared and their individual characteristics analyzed. The chapter reveals why the comparison of a sensor evaluated in two different clinical studies is not always straightforward.

The chapter “Can We Use Measurements to Classify Patients Suffering from Type 1 Diabetes into Subcategories and Does It Make Sense?” by Florian Reiterer et al. makes use of continuous time prediction models to describe the interaction between ingested carbohydrates, subcutaneously injected insulin, and continuously measured glucose concentration. The identified model parameters of 12 subjects were analyzed and statistically significant correlations between the parameters and patient characteristics such as weight and age could be found.

The chapter “Prevention of Severe Hypoglycemia by Continuous EEG Monitoring” by Claus Borg Juhl et al. shows how to use EEG signals to predict upcoming hypoglycemic situations in real-time by employing artificial neural networks. The results of a 30-day long clinical study with the implanted device and the developed algorithm are presented.

The chapter “Meta-Learning Based Blood Glucose Predictor for DiabeticSmartphone App” by Valeriya Naumova et al. demonstrates how a highly sophisticated glucose prediction model can be ported from a development language running on a PC to a format such that it can be used conveniently by the patients. A unique feature of the algorithm is its independence of any user input other than historic CGM data which is automatically transmitted from a CGM device. No parameter estimation nor prediction model individualization is required.

The chapter “Predicting Glycemia in Type 1 Diabetes Mellitus with Subspace-Based Linear Multistep Predictors” by Marzia Cescon et al. uses data-based methods to develop individualized prediction models. The model can be considered as a combination of physiological models to precompute the rate of appearance of injected insulin and ingested carbohydrates in the bloodstream and of data-based models to combine this information and compute predictions up to 120 min in the future. The results show the performance on data from 14 type 1 diabetes patients in a clinical trial.

The chapter “Empirical Representation of Blood Glucose Variability in a Compartmental Model” by Stephen D. Patek et al. shows a modeling technique designed to extract the information on the net effect of meals on the blood glucose concentration. By assuming that all major unexplained glycemic excursions can be vi Preface attributed to oral glucose ingestion, a meal vector is estimated which significantly improves the mathematical model. Results are shown on three patients during a clinical trial and on virtual patients where it is shown how the method can be used for adjustments of the basal insulin rate.

The chapter “Physiology-Based Interval Models: A Framework for Glucose Prediction Under Intra-patient Variability” by Jorge Bondia and Josep Vehi tries to cope with the large intrasubject variability by using the concept of interval predictions. Instead of predicting a single blood glucose value in the future, a whole solution envelope is determined. With the presented theory it can be guaranteed that the real value is always inside of the envelope and moreover the envelope is not conservative. The method is evaluated on a physiological diabetes model.

The chapter “Modeling and Prediction Using Stochastic Differential Equations” by Rune Juhl et al. considers uncertainty in the dynamics between different patients as well as within a patient by making use of stochastic differential equations. It is shown how the mixed effects modeling methodology can be applied such that the underlying information of several datasets from different patients is extracted to form the model.

The chapter “Uncertainties and Modeling Errors of Type 1 Diabetes Models” by Levente Kovács and Péter Szalay analyzes the effect of prediction model uncertainties on the control system during a design procedure involving the steps model reduction by elimination of state variables, state estimation using extended Kalman Filters and Sigma Point filters and linear parameter-varying control synthesis.
The chapter "Recent Results on Glucose–Insulin Predictions by Means of a State Observer for Time-Delay Systems" by Pasquale Palumbo et al. introduces a prediction model which in real time predicts the insulin concentration in blood which in turn is used in a control system. The method is tested in simulation on a time-delay system representing the glucose–insulin system.

The chapter "Performance Assessment of Model-Based Artificial Pancreas Control Systems" by Jianyuan Feng et al. makes use of prediction models to compute treatment advices. The novelty of the proposed algorithm consists in explicitly considering (among others) the model prediction error and model error elimination speed. A retuning of the advisory system is done in case the prediction model does not perform well. Results on 30 virtual patients show the performance of the control system.

We would like to thank all people involved in the process of writing this book: All authors for their individual contributions, all reviewers of the book chapters, Daniela Hummer for the entire organization of the workshop, Boris Tasevski for helping with the typesetting, Florian Reiterer for his help editing the book, as well as Oliver Jackson and Karin de Bie for the good cooperation with Springer.
same rock material was used to illustrate the use of low field NMR to detect differences in the texture of chalk; in our case in single cases; therefore, it is doubtful whether it is the responsible mechanism for the water weakening of chalk. The detect any precipitation that may occur in the pore space of chalk saturated with divalent ions. Precipitation occurred only and pore collapse of this rock was observed and validated from the ultrasonic velocity data. Low field NMR was used to concentration on the chalk surface; such as precipitation and dissolution. The effect of the divalent ions on the elasticity for rock mechanical testing in order to understand the potential mechanisms behind the action of ions in high Chalk from Stevns Klint near Copenhagen, Denmark, (a rock analogue to reservoir chalk from the North Sea) was used rock samples.

advanced experiments are performed; X-ray diffraction (XRD), backscatter electron microscopy images (BSEM), mercury injection capillary pressure (MICP) curves and specific surface analysis (BET) illustrate the mineralogy and texture of the rock samples. Chalk from Stevns Klint near Copenhagen, Denmark, (a rock analogue to reservoir chalk from the North Sea) was used for rock mechanical testing in order to understand the potential mechanisms behind the action of ions in high concentration on the chalk surface; such as precipitation and dissolution. The effect of the divalent ions on the elasticity and pore collapse of this rock was observed and validated from the ultrasonic velocity data. Low field NMR was used to detect any precipitation that may occur in the pore space of chalk saturated with divalent ions. Precipitation occurred only in single cases; therefore, it is doubtful whether it is the responsible mechanism for the water weakening of chalk. The same rock material was used to illustrate the use of low field NMR to detect differences in the texture of chalk; in our case
a carbonate mudstone and a carbonate wackestone as previously observed by electron microscopy. The solid-fluid affinity of chalk from the Gorm field, Berea sandstone and chlorite bearing greensand from the Solsort field was defined from low field NMR data. Longitudinal relaxation time (T1), transverse relaxation time (T2) and self-diffusion coefficient of the fluids within the core plugs were measured at different saturation states; water, reservoir oil and oil and water at irreducible water saturation. T1/T2 ratio proved a non-destructive and fast way to determine the solid-fluid affinity and fluid distribution within the pore space of the selected rocks. Finally, supplementary experimental work includes the determination of small amounts of oil in water samples from the NMR T2 distribution. Low field NMR spectrometry was able to accurately determine the oil and water volume in effluents. This is found very useful, because when the oil reaches residual saturation during core flooding experiments, the produced oil is very small and the quantification of these fluids is often difficult.

General information
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Organisations: Department of Civil Engineering, Section for Geotechnics and Geology, Center for Energy Resources Engineering
Authors: Katika, K. (Intern), Fabricius, I. L. (Intern)
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Publication date: 2016

Publication information
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Original language: English

Simulation and multivariable optimization of post-combustion capture using piperazine
Piperazine presents a great potential to develop an energy efficient solvent based CO2 post-combustion capture process. Recently 8 molal piperazine (PZ) has shown promising results, however it faces operational challenges due to limited solid solubility. The operating range can be extended by decreasing the concentration of PZ and/or increasing the lean loading. However, optimal process conditions must be determined accounting for heating and cooling demands plus solvent recirculation. In this paper, we identify and generalize trends of performance for a broad range of operating conditions: 1.8-9 m PZ/kg water (molal) and 0.2-0.6 lean loading for absorption and desorption in both, open and closed-loop simulation. We pinpoint scenarios where intercooling significantly improves the performance of the post-combustion process. The energy penalty is minimized as part of the closed-loop multivariable optimization. The results are created in Aspen Plus using the hybrid CAPCO2 rate-based user model. This model includes precipitation when estimating the heat and mass transfer rates. The results show how the capture process needs to be operated up to 14% above the minimum achievable heat duty, to avoid clogging from solid formation. 5 m PZ is the most promising trade-off between energy efficiency and solid-free operation with a specific reboiler duty of 3.22 GJ/t CO2 at 0.34 lean loading. The performance of the process can be further improved by assuming a minimum temperature of 30 °C which gives an optimal specific reboiler duty of 3.09 GJ/t CO2 (8 m PZ, 0.334 lean loading) for conditions without advanced heat integration.

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Solubility modeling in the binary system Fe(NO₃)₃–H₂O, Co(NO₃)₂–H₂O and the ternary system Fe(NO₃)₃–Co(NO₃)₂–H₂O is presented. The extended UNIQUAC model was applied to the thermodynamic assessment of the investigated systems. The model parameters obtained were regressed simultaneously using the available databank but with more experimental points, recently published in the open literature. A revision of previously published parameters for the cobalt ion and new parameters for the iron(III) nitrate system are presented. Based on this set of parameters, the equilibrium constants of hydrates are determined. The model represents the experimental data with good accuracy from the freezing point region to the boiling points of the solutions.

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Organisations: Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering, University Hassan I
Authors: Arrad, M. (Ekstern), Kaddami, M. (Ekstern), Goundali, B. E. (Ekstern), Thomsen, K. (Intern)
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Publication information
The Phase Envelope of Multicomponent Mixtures in the Presence of a Capillary Pressure Difference

Confined fluids such as oil and gas mixtures inside tight reservoirs are systems that can experience high capillary pressure difference between the liquid and gas phases. This capillary pressure difference has an effect on the phase equilibrium and in some cases is considerably high. We presented an algorithm which can reliably compute the whole phase envelope for multicomponent mixtures when there is a capillary pressure difference. It uses an equation of state for the phase equilibrium and the Young-Laplace equation for the capillary pressure model. The algorithm proves to be robust...
and efficient for test mixtures with wide ranges of compositions at different capillary radii and vapor fractions. The calculation results show that the phase envelope changes everywhere except at the critical point. The bubble point and the lower branch of the dew point show a decrease in the saturation pressure, whereas the upper branch of the dew point shows an increase. The cricondentherm is shifted to a higher temperature. We also presented a mathematical analysis of the phase envelope shift due to capillary pressure based on linear approximations. The resulting linear approximation equations can predict the correct direction of the phase envelope shift. Combined with the multicomponent Clapeyron equation, the equations reveal why the shift changes direction for the saturation pressure at the cricondentherm and for the saturation temperature at the cricondenbar. The equations can be used to estimate the magnitude of shift, and the approximation is close for the change in the bubble point pressure.
Time-explicit methods for joint economical and geological risk mitigation in production optimization

Real-life applications of production optimization face challenges of risks related to unpredictable fluctuations in oil prices and sparse geological data. Consequently, operating companies are reluctant to adopt model-based production optimization into their operations. Conventional production optimization methods focus on mitigation of geological risks related to the long-term net present value (NPV). A major drawback of such methods is that the time-dependent and exceedingly growing uncertainty of oil prices implies that long-term predictions become highly unreliable. Conventional methods therefore leave the oil production subject to substantial economical risk. To address this challenge, this paper introduces a novel set of time-explicit (TE) methods, which combine ideas of multi-objective optimization and ensemble-based risk mitigation into a computationally tractable joint effort of mitigating economical and geological risks. As opposed to conventional strategies that focus on a single long-term objective, TE methods seek to reduce risks and promote returns over the entire reservoir life by optimization of a given ensemble-based geological risk measure over time. By explicit involvement of time, economical risks are implicitly addressed by balancing short-term and long-term objectives throughout the reservoir life. Open-loop simulations of a two-phase synthetic reservoir demonstrate that TE methods may significantly improve short-term risk measures such as expected return, standard deviation and conditional value-at-risk compared to nominal, robust and mean-variance optimization. The gains in short-term objectives are obtained with none or only slight deterioration of long-term objectives.

General information
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Organisations: Center for Energy Resources Engineering, Department of Applied Mathematics and Computer Science, Scientific Computing
Authors: Christiansen, L. H. (Intern), Capolei, A. (Intern), Jørgensen, J. B. (Intern)
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Main Research Area: Technical/natural sciences

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We introduce a new stabilized high-order and unstructured numerical model for modeling fully nonlinear and dispersive water waves. The model is based on a nodal spectral element method of arbitrary order in space and a -transformed formulation due to Cai, Langtangen, Nielsen and Tveito (1998). In the present paper we use a single layer of quadratic (in 2D) and prismatic (in 3D) elements. The model has been stabilized through a combination of over-integration of the
Galerkin projections and a mild modal filter. We present numerical tests of nonlinear waves serving as a proof-of-concept validation for this new high-order model. The model is shown to exhibit exponential convergence even for very steep waves and there is a good agreement to analytic and experimental data.

**General information**

State: Published

Organisations: Center for Energy Resources Engineering, Department of Applied Mathematics and Computer Science, Scientific Computing, Massachusetts Institute of Technology, Chalmers University of Technology

Authors: Engsig-Karup, A. P. (Intern), Eskilsson, C. (Ekstern), Bigoni, D. (Ekstern)

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**Videnskabelig udredning af international viden om skifergas relateret til en dansk kontekst: DTU, GEUS, DCE**

**General information**

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Organisations: Office for Innovation & Sector Services, Department of Environmental Engineering, Department of Civil Engineering, Environmental Chemistry, Water Resources Engineering, Section for Geotechnics and Geology, Center for Energy Resources Engineering, Section for Building Design, Residual Resource Engineering, Water Technologies, Production and Service Management, Department of Management Engineering, Engineering Systems, Department of Transport, Transport policy and behaviour, Geological Survey of Denmark and Greenland, Aarhus University, DCE - National Center for Miljø og Energi, Geological Survey of Denmark


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**Wettability of chalk and argillaceous sandstones assessed from T1/T2 ratio**
A Bolus Calculator Based on Continuous-Discrete Unscented Kalman Filtering for Type 1 Diabetics

In patients with type 1 diabetes, the effects of meals intake on blood glucose level are usually mitigated by administering a large amount of insulin (bolus) at mealtime or even slightly before. This strategy assumes, among other things, a prior knowledge of the meal size and the postprandial glucose dynamics. On the other hand, administering the meal bolus during or after mealtime could benefit from the information provided by the postprandial meal dynamics at the expense of a delayed meal bolus. The present paper investigates different bolus administration strategies (at mealtime, 15 minutes after or 30 minutes after the beginning of the meal). We implement a continuous-discrete unscented Kalman filter to estimate the states and insulin sensitivity. These estimates are used in a bolus calculator. The numerical results demonstrate that administering the meal bolus 15 minutes after mealtime both reduces the risk of hypoglycemia in case of an overestimated meal and the time spent in hyperglycemia if the meal size is underestimated. Faster insulin and the use of glucagon will have the potential to encourage postprandial meal bolus administration and hence will not require to accurately estimate the meal size.
A Continuous-Discrete Extended Kalman Filter for State and Parameter Estimation in People with Type 1 Diabetes

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Organisations: Department of Applied Mathematics and Computer Science, Scientific Computing, Dynamical Systems, Center for Energy Resources Engineering, Slovak University of Technology, Technical University of Denmark, Copenhagen University Hospital
Number of pages: 1
Publication date: 2015
Main Research Area: Technical/natural sciences

A general enhancement factor model for absorption and desorption systems: A CO₂ capture case-study
This study derives a general method (GM) for reactive absorption and desorption calculation. It connects the Onda's approximation for reversible reactions with the van Krevelen's approach for instantaneous irreversible reactions. It is set-up for a reversible (m+n)-th order, forward reaction kinetics and applied for the CO₂-MEA-H₂O second order reversible system. The results show that the GM predicts the two-film theory within 2% accuracy and the surface renewal model within 10% accuracy, both at absorber and desorber conditions and for high driving force and pinch conditions. GM is compared to the ideas of van Krevelen, and Astarita and Savage. An analysis demonstrates how the GM model eliminates many of the limitations of previous approaches. It has a noticeable potential to enhance the accuracy of process simulators without sacrificing the simulation time. It could eliminate the need for conservative and uncertain design and therefore it will lead to more realistic cost estimations.

General information
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Organisations: Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering, CERE – Center for Energy Ressources Engineering
Authors: Gaspar, J. (Intern), Fosbøl, P. L. (Intern)
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We develop an efficient homogeneous and self-dual interior-point method (IPM) for the linear programs arising in economic model predictive control of constrained linear systems with linear objective functions. The algorithm is based on a Riccati iteration procedure, which is adapted to the linear system of equations solved in homogeneous and self-dual IPMs. Fast convergence is further achieved using a warm-start strategy. We implement the algorithm in MATLAB and C. Its performance is tested using a conceptual power management case study. Closed loop simulations show that 1) the proposed algorithm is significantly faster than several state-of-the-art IPMs based on sparse linear algebra, and 2) warm-start reduces the average number of iterations by 35-40%.
An electrolyte CPA equation of state for mixed solvent electrolytes

Despite great efforts over the past decades, thermodynamic modeling of electrolytes in mixed solvents is still a challenge today. The existing modeling frameworks based on activity coefficient models are data-driven and require expert knowledge to be parameterized. It has been suggested that the predictive capabilities could be improved through the development of an electrolyte equation of state. In this work, the Cubic Plus Association (CPA) Equation of State is extended to handle mixtures containing electrolytes by including the electrostatic contributions from the Debye-Hückel and Born terms using a self-consistent model for the static permittivity. A simple scheme for parameterization of salts with a limited number of parameters is proposed and model parameters for a range of salts are determined from experimental data of activity and osmotic coefficients as well as freezing point depression. Finally, the model is applied to predict VLE, LLE, and SLE in aqueous salt mixtures as well as in mixed solvents.

General information
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Organisations: CERE – Center for Energy Resources Engineering, Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering
Authors: Maribo-Mogensen, B. (Intern), Thomsen, K. (Intern), Kontogeorgis, G. M. (Intern)
Number of pages: 18
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Main Research Area: Technical/natural sciences

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Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.11 SJR 1.034 SNIP 1.268
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.085 SNIP 1.417 CiteScore 3.03
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.07 SNIP 1.332 CiteScore 2.86
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.05 SNIP 1.364 CiteScore 2.59
ISI indexed (2013): ISI indexed yes
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BFI (2012): BFI-level 2
Scopus rating (2012): SJR 0.989 SNIP 1.437 CiteScore 2.46
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Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.004 SNIP 1.234 CiteScore 2.31
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.083 SNIP 1.423
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.192 SNIP 1.437
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 1.287 SNIP 1.428
Web of Science (2008): Indexed yes
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Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.483 SNIP 1.612
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.309 SNIP 1.64
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Scopus rating (2004): SJR 1.297 SNIP 1.654
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 1.694 SNIP 1.578
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 1.749 SNIP 1.725
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 2.16 SNIP 2.077
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 1.953 SNIP 1.76
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DOIs:
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Publication: Research - peer-review › Journal article – Annual report year: 2015

Bi-hormonal Closed-loop Control of Blood Glucose for People With Type 1 Diabetes - the Diacon Project

General information
State: Published
Organisations: Department of Applied Mathematics and Computer Science , Scientific Computing, Dynamical Systems, Center for Energy Resources Engineering, Copenhagen University Hospital, Slovak University of Technology
Brine crude oil interactions at the oil-water interface
The impact of brine salinity and its ionic composition on oil displacement efficiency has been investigated extensively in recent years due to the potential of enhanced oil recovery (EOR). Wettability alterations through relative interactions at the mineral surface have been the basis of proposed mechanisms. The ion specific interaction between fines and polar fractions of crude oil at the oil-water interface was determined. The experiments prove the importance of Ca\(^{2+}\), SO\(_4^{2-}\), and HPO\(_4^{2-}\) ions in enhancing oil emulsion formation by increasing interactions between polar acids and brine solutions. The results propose the potential use of HPO\(_4^{2-}\) ions in reservoirs having inactive mineral surfaces. The relative oil affinity of different ions including K\(^+\), Na\(^+\), Mg\(^{2+}\), and Ca\(^{2+}\) (cations), and Cl\(^-\), SO\(_4^{2-}\), HPO\(_4^{2-}\), and HCO\(_3^{-}\) (anions), were studied through gas chromatographic analysis. Crude oil from the North Sea was doped with various fractions of organic acids to mimic different polar behavior. Increased brine concentration showed up to 15% upsurge of polar fractions on the oil-water emulsion formation. During emulsion formation the relative interactions at the oil-water interface are proved to follow the Hofmeister series: K\(^+\)<Na\(^+\)<Mg\(^{2+}\)<Ca\(^{2+}\). Beyond CaCl\(_2\) concentrations of 0.08 mol/l no additional acid participation in emulsion formation was observed. Among anions, SO\(_4^{2-}\) and HPO\(_4^{2-}\) showed optimum emulsion formation at 0.05 mol/l. The amount of emulsion formation showed significant dependency on the type of acid doped in oil. Experiments demonstrate that the brine solution can alter the micro forces at the oil-water interface, and this ion specific interaction leads to oil emulsion formation and thus reduces the interfacial viscoelasticity of the trapped oil. These results show significant correlation between oil emulsion formation and increased oil recovery. Copyright 2015; Society of Petroleum Engineers

Characterization Scheme for Property Prediction of Fluid Fractions Originating from Biomass
The composition of industrial fluids is often very difficult to identify from the molecular point of view. In the petroleum industry, the use of the so-called “pseudo-components” is commonly accepted in process modeling, and various approaches exist to determine and/or construct them. We have identified and summarized four such approaches, generally based on experimental information such as boiling temperature and density. Fluids that originate from biomass, however, cannot be treated using only volatility, because of the highly polar character and the high molecular weight of its components, resulting in highly nonideal phase equilibrium behavior. In this work, it is proposed to use a more complete set of experimental descriptors in order to determine the chemical structure of an unknown fluid cut. The definition of such a representative molecule (surrogate) makes it possible to use group contribution or other predictive tools for property calculations or characteristic parameters of an equation of state. In order to achieve this goal, a large database of monofunctional molecules (including alcohols, n-aliphatic acids, aldehydes, ketones, aliphatic ethers, esters, n-alkylbenzenes, and alkanes) has been constructed, which contains a number of descriptors originating from analytical measurements. Using physical insight on the molecular interactions, an algorithm is proposed that uses five descriptors (molecular weight, liquid molar volume, viscosity, refractive index, and dielectric constant) in order to reconstruct a representative molecule.
Comparison of Linear and Nonlinear Model Predictive Control for Optimization of Spray Dryer Operation

In this paper, we compare the performance of an economically optimizing Nonlinear Model Predictive Controller (E-NMPC) to a linear tracking Model Predictive Controller (MPC) for a spray drying plant. We find in this simulation study, that the economic performance of the two controllers are almost equal. We evaluate the economic performance with an industrially recorded disturbance scenario, where unmeasured disturbances and model mismatch are present. The state of the spray dryer is...
Comparison of Prediction Models for a Dual-Hormone Artificial Pancreas

In this paper we compare the performance of five different continuous time transfer function models used in closed-loop model predictive control (MPC). These models describe the glucose-insulin and glucose-glucagon dynamics. They are discretized into a state-space description and used as prediction models in the MPC algorithm. We simulate a scenario including meals and daily variations in the model parameters. The numerical results do not show significant changes in the glucose traces for any of the models, excepted for the first order model. From the present study, we can conclude that the second order model without delay should provide the best trade-off between sensitivity to uncertainties and practical usability for in vivo clinical studies.
This paper presents a mixed-integer linear optimization problem for unit commitment and economic dispatch of power generators in a meshed isolated power system. The optimization problem is referred to as the optimal reserve planning problem (ORPP). The ORPP guarantees that the system frequency is kept above a predefined limit in the event of a contingency. The minimum frequency constraints are formulated using novel sufficient conditions that take into account the system inertia and the dynamics of the power generators. The proposed sufficient conditions are attractive from both a computational and a modelling point of view. We compare the ORPP to a unit commitment problem that only considers the stationary behavior of the frequency. Simulations based on a Faroe Islands case study show that, without being overly conservative, potential blackouts and power outages can be avoided using the ORPP. In the particular case study, the cost increase associated with the additional security provided by the ORPP is less than 3%.
Dynamic and flexible operation of a carbon capture plant is important as thermal power plants must be operated very flexibly to accommodate large shares of intermittent energy sources such as wind and solar energy. To facilitate such operation, dynamic models for simulation, optimization and control system design are crucial. In this paper, we present a dynamic mathematical model for the absorption and desorption columns in a carbon capture plant. Moreover, we implement a decentralized proportional-integral (PI) based control scheme and we evaluate the performance of the control
structure for various operational procedures, e.g. start-up, load changes, noise on the flue gas flow rate and composition. Note that the carbon capture plant is based on the solvent storage configuration. To the authors knowledge, this is the first paper addressing the issue of start-up operation and control of carbon capture. The study demonstrates that the implemented control structure keeps the carbon capture process at 90% CO2 removal rate with a deviation up to 8% during load variations. In addition, it reveals that the control structure brings the process to the desired set point in approximately 10 min during process start-up.

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- **Authors:** Gaspar, J. (Intern), Jørgensen, J. B. (Intern), Fosbøl, P. L. (Intern)
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**Control of Electricity Loads in Future Electric Energy Systems**

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- **Organisations:** Centre for IT-Intelligent Energy Systems in Cities, Department of Applied Mathematics and Computer Science, Dynamical Systems, Scientific Computing, Center for Energy Resources Engineering, DONG Energy A/S
- **Authors:** Madsen, H. (Intern), Parvizi, J. (Intern), Halvgaard, R. F. (Intern), Sokoler, L. E. (Intern), Jørgensen, J. B. (Intern), Hansen, L. H. (Intern), Hilger, K. B. (Intern)
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- **ISBN (Print):** 978-1-118-38858-7
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- **Main Research Area:** Technical/natural sciences
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**Cubic Plus Association Equation of State for Flow Assurance Projects**

Thermodynamic hydrate inhibitors such as methanol, ethanol, (mono) ethylene glycol (MEG), and triethylene glycol (TEG) are widely used in the oil and gas industry. On modeling these compounds, we show here how the CPA equation of state was implemented in an in-house process simulator as an in-built model: To validate the implementation, we show calculations for binary systems containing hydrate inhibitors and water or hydrocarbons using the Cubic Plus Association (CPA) and Soave-Redlich-Kwong (SRK) equation of states, also comparing against experimental data. For streams containing natural gas and water, CPA was applied to calculate the loss of the inhibitor to the vapor phase as a function of temperature and pressure. Simulations of dehydration units using TEG were conducted, and the CPA results were compared with that of two commercial simulators which used their available thermodynamic packages for glycol applications, proving that the CPA calculations are in good agreement with these models and showing that this is an adequate way to simulate complex matures containing natural gas, water, and hydrate inhibitors.
Densities of the Binary Systems n-Hexane + n-Decane and n-Hexane + n-Hexadecane up to 60 MPa and 463 K

The densities of the binary systems n-hexane + n-decane and n-hexane + n-hexadecane have been measured up to 60 MPa using a vibrating tube densimeter. The measurements covered the whole composition range; for the first system they were performed from (278.15 to 463.15) K, while for the latter they were performed from (298.15 to 463.15) K because n-hexadecane is a solid at 278.15 K. The densities were correlated for every composition as a function of temperature and pressure using a modified Tammann-Tait equation with standard deviations lower than 8·10-4 g·cm-3. Isothermal compressibility values were calculated from the experimental density data. Moreover, the excess volumes were found to be negative for all of the studied mixtures, with absolute values less than or equal to 3.25 cm3·mol-1 for the n-hexane + n-decane system and 7.65 cm3·mol-1 for the n-hexane + n-hexadecane system. Various equations of state were used to model the measured density data.

General information

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Determination of asphaltene onset conditions using the cubic plus association equation of state

The cubic-plus-association (CPA) equation of state (EoS) has already been proven to be a successful model for phase equilibrium calculations for systems containing associating components and has already been applied for asphaltene modeling by few researchers. In the present work, we apply the CPA EoS to determine asphaltene precipitation onset conditions for various reservoir fluids but with a different modeling approach than literature approaches. A simple oil characterization technique, based on SARA analysis, is adopted which divides the C6+ fraction of the oil into “heavy component” and asphaltene. Self-association between asphaltene molecules and cross-association between asphaltene and heavy component molecules are considered. Experimental data of several reservoir fluids are compared with model results and it is found that the temperature dependent cross-association energy correlates asphaltene phase envelope quite well in agreement with the experimental data. Two experimental asphaltene onset points at different temperatures and one bubble point data of reservoir fluid are required in order to determine the temperature dependent cross-association energy and critical pressure of heavy component respectively. The effect of gas injection on asphaltene precipitation is also correlated with experimental data by tuning a single binary interaction parameter of the injected gas...
component and asphaltene pair.

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Organisations: Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering
Authors: Arya, A. (Intern), von Solms, N. (Intern), Kontogeorgis, G. M. (Intern)
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- Scopus rating (2013): SJR 1.007 SNIP 1.274 CiteScore 2.31
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- Web of Science (2011): Indexed yes
- BFI (2010): BFI-level 2
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- Web of Science (2010): Indexed yes
- BFI (2009): BFI-level 2
- Scopus rating (2009): SJR 1.133 SNIP 1.164
- Web of Science (2009): Indexed yes
- BFI (2008): BFI-level 1
- Scopus rating (2008): SJR 1.227 SNIP 1.09
- Web of Science (2008): Indexed yes
- Scopus rating (2007): SJR 1.031 SNIP 1.151
- Web of Science (2007): Indexed yes
- Scopus rating (2006): SJR 1.034 SNIP 1.245
- Web of Science (2006): Indexed yes
- Scopus rating (2005): SJR 1.009 SNIP 1.3
- Web of Science (2005): Indexed yes
Different effects of temperature and salinity on permeability reduction by fines migration in Berea sandstone

Hot water injection into geothermal aquifers is considered in order to store energy seasonally. Berea sandstone is often used as a reference formation to study mechanisms that affect permeability in reservoir sandstones. Both heating of the pore fluid and reduction of the pore fluid salinity can reduce permeability in Berea sandstone. These effects could be caused by mobilisation of fines by increasing the repulsive electrical double layer forces among sandstone grains and the fines. We investigated the reversibility and the dependence on flow velocity and flow direction of the permeability change by means of flow through experiments and examined thin sections of samples prior to and after tests. A permeability reduction at 20 degrees C with decreasing salinity was not reversed by restoring the salinity, whereas a permeability reduction due to heating to 80 degrees C was reversible by restoring the temperature to 20 degrees C. A reversible permeability increase with increasing flow rate was observed at 80 degrees c but not at 20 degrees C. We observed no difference in the distribution of kaolinite clay minerals in thin section of untested and tested samples. Dissolution of iron bearing carbonates and precipitation of iron hydroxides was observed but no effect on permeability was found. The experimental results suggest that different mechanisms are responsible for permeability reduction depending on temperature and salinity. (C) 2014 Elsevier Ltd. All rights reserved.

General information
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Organisations: Department of Civil Engineering, Section for Geotechnics and Geology, Center for Energy Resources Engineering, Geological Survey of Denmark and Greenland, Technical University of Denmark, University of Leeds
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Scopus rating (2015): SJR 1.344 SNIP 1.987 CiteScore 2.99
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
In this thesis, we consider control strategies for large and distributed energy systems that are important for the implementation of smart grid technologies. An electrical grid has to ensure reliability and avoid long-term interruptions in the power supply. Moreover, the share of Renewable Energy Sources (RESs) in the smart grids is increasing. These energy sources bring uncertainty to the production due to their fluctuations. Hence, smart grids need suitable control systems that are able to continuously balance power production and consumption. We apply the Economic Model Predictive Control (EMPC) strategy to optimise the economic performances of the energy systems and to balance the power production and consumption. In the case of large-scale energy systems, the electrical grid connects a high number of power units. Because of this, the related control problem involves a high number of variables and constraints and its solution requires high computational times. Energy systems have a hierarchical control framework and the controllers have to work in the time-scale required by their hierarchy level. Dedicated optimisation techniques efficiently solve the control problem and reduce computational time. We implement the Dantzig-Wolfe decomposition technique to efficiently solve the EMPC problem.

The contributions of this thesis are primarily on:

**Large-scale energy system**

Smart-grids connect a high number of energy units. In such a large-scale scenario the energy units are independent and dynamically decoupled. The mathematical model of the large-scale energy system embodies the decoupled dynamics of each power unit. Moreover, all units of the grid contribute to the overall power production.

**Economic Model Predictive Control (EMPC)**

This control strategy is an extension of the Model Predictive Control (MPC) strategy. Energy systems often involve stochastic variables due to the share of fluctuating Renewable Energy Sources (RESs). Moreover, the related control problems are multi variables and they are hard, or impossible, to split into single-input-single-output control systems. MPC strategy can handle multi variables control problems and it can embody stochastic variables. The Economic MPC (EMPC)
policy optimises the economic performances of the process. In this work, we apply the EMPC to energy systems and it computes the control trajectory for each energy unit. This control policy minimises production costs and ensures that the power production satisfies the customers’ demand. The EMPC designs a linear control problem that has a block-angular constraints matrix and it has two sets of constraints. The independent dynamics of the energy units define the decoupling constraints sited on the diagonal. The coupling constraints represent the common goal of all power units in the energy system and this is to satisfy the customers’ demand. The Dantzig-Wolfe optimisation technique applies to this structure of the constraints matrix in the view of fastening the control algorithm and increase its applicability.

**Dantzig-Wolfe decomposition**

The Dantzig-Wolfe decomposition solves the EMPC problem through a distributed optimisation technique. The EMPC problem via Dantzig-Wolfe decomposition algorithm computes the optimal input trajectory for each energy unit and reduces the computation times. Moreover, such a control algorithm applies to large-scale energy systems and the number of energy units does not affect the performances of the controller. In this thesis, we also investigate suboptimal solutions of the EMPC problem via modified versions of the Dantzig-Wolfe decomposition algorithms. The feasibility of the suboptimal solutions suffices for stability. The goal of these modified Dantzig-Wolfe decomposition algorithms is to reduce computation time in the solution of the EMPC problem.

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**Economic Optimization of Spray Dryer Operation using Nonlinear Model Predictive Control with State Estimation**

In this paper, we develop an economically optimizing Nonlinear Model Predictive Controller (E-NMPC) for a complete spray drying plant with multiple stages. In the E-NMPC the initial state is estimated by an extended Kalman Filter (EKF) with noise covariances estimated by an autocovariance least squares method (ALS). We present a model for the spray drying plant and use this model for simulation as well as for prediction in the E-NMPC. The open-loop optimal control problem in the E-NMPC is solved using the single-shooting method combined with a quasi-Newton Sequential Quadratic programming (SQP) algorithm and the adjoint method for computation of gradients. We evaluate the economic performance when unmeasured disturbances are present. By simulation, we demonstrate that the E-NMPC improves the profit of spray drying by 17% compared to conventional PI control.

**General information**

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Organisations: Department of Applied Mathematics and Computer Science, Scientific Computing, Center for Energy Resources Engineering, University of Wisconsin-Madison
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Efficient solvers for soft-constrained MPC

In this work, integrated design and control of reactive distillation processes is presented. Simple graphical design methods that are similar in concept to non-reactive distillation processes are used, such as reactive McCabe-Thiele method and driving force approach. The methods are based on the element concept, which is used to translate a system of compounds into elements. The operation of the reactive distillation column at the highest driving force and other candidate points is analyzed through analytical solution as well as rigorous open-loop and closed-loop simulations. By application of this approach, it is shown that designing the reactive distillation process at the maximum driving force results in an optimal design in terms of controllability and operability. It is verified that the reactive distillation design option is less sensitive to the disturbances in the feed at the highest driving force and has the inherent ability to reject disturbances.

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Electrical tortuosity, Kozeny’s factor and cementation factor modelled for chalk

Based on the electrical properties of chalk from the North Sea and Stevns Klint and on published data, we explore how klinkenberg corrected permeability from experimental data relate to porosity and electrical resistivity. In the current study we use electrical conductivity data of partially water saturated core plugs to determine the cementation factor, $m$. This value differs from the one Archie used to describe his equation and best describes the formation factor based on experimental data. Based on this $m$, we determine the formation factor, $F$, and the tortuosity, $\tau$. We use this value of $\tau$, to calculate permeability based on electrical resistivity data. We also calculate the permeability based on a simple porosity model. Finally, we redefine Kozeny’s factor, $\kappa$, using Carman’s model based on tortuosity and the model based on porosity. This resulted in a third modelled permeability, which describes the experimental data in high accuracy.

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Experimental validation of kinetic inhibitor strength on natural gas hydrate nucleation

The kinetics of natural gas hydrate formation in the presence of dissolved salts (NaCl) and crude oil (a middle east crude with density 851.5 kg/m$^3$) were investigated by using a standard rocking cell (RC-5) apparatus. The hydrate nucleation temperature was reduced in the presence of NaCl and oil in comparison with that in pure distilled water. The kinetic inhibition strength of various inhibitors (Luvicap Bio; Inhibex 505; Inhibex 501; Luvicap 55w; BIO inhibex-800; and Inhibex 301) was experimentally evaluated at complex conditions (in the presence of salts and crude oil) using the constant cooling temperature approach. These polymer-based chemicals were ranked based on the inhibition strength as follows: Luvicap Bio < Inhibex 505 < Luvicap 55w < Inhibex 501 < BIO-Inhibex-800 < Inhibex 301. The same trend was also observed
in the presence of salts and liquid hydrocarbon phase. The KHIs' inhibition strength was not affected by NaCl but decreased significantly in the presence of crude oil. The hydrate decomposition temperatures were not influenced by the presence of NaCl, however, they decreased slightly in the presence of liquid hydrocarbon. The data presented here can contribute to appropriate hydrate risk management in oil and gas facilities. (C) 2014 Elsevier Ltd. All rights reserved.

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Scopus rating (2010): SJR 1.984 SNIP 2.319  
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Scopus rating (2009): SJR 2.012 SNIP 2.277  
Web of Science (2009): Indexed yes  
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Scopus rating (2008): SJR 1.635 SNIP 2.184  
Web of Science (2008): Indexed yes  
Scopus rating (2007): SJR 1.383 SNIP 1.86  
Web of Science (2007): Indexed yes  
Scopus rating (2006): SJR 1.278 SNIP 1.64  
Web of Science (2006): Indexed yes
Extracurricular scientific production among medical students has increased in the past decade

Introduction: Undergraduate research among medical students is essential in the education of future physicians and scientists. This study aimed to evaluate the scientific yield of extracurricular undergraduate research among medical students. Methods: Medical students at the University of Copenhagen who completed an extracurricular research year between January 2004 and June 2013 were evaluated through a manual search in PubMed MEDLINE. The primary focus was the number of peer-reviewed, published articles. Results: Of the 363 included students, 3.1% did their research in 2004-2005 compared with 46.5% in 2012-2013. After three years, 70.4% of the students had published a peer-reviewed article; and of all the 363 students, 36.5% had published as a first author. In total, 87.7% had a medical specialty as their research area versus a surgical specialty. Cardiology was also associated with the greatest scientific yield with a median number of 0.8 publications per year after the students concluded their undergraduate research period. Three or more years after concluding their undergraduate research, 32.8% of the students had continued with research in the context of a PhD programme. Conclusion: Overall, the number of medical students who engage in extracurricular research follows an increasing trend, and more than two-thirds of these students publish a peer-reviewed paper within three years. Cardiology was the most popular specialty and also the specialty with the greatest scientific yield. A third of the undergraduate research students continued doing research in the context of a PhD programme.
Fine Formation During Brine-Crude Oil-Calcite Interaction in Smart Water Enhanced Oil Recovery for Caspian Carbonates

Modified sea water has been shown to affect the oil recovery fraction considerably during secondary and tertiary waterfloods. Available soluble potential ions (i.e. Ca$^{2+}$, Mg$^{2+}$ & SO$_{4}^{2-}$) in the interacting waterflood (ITW) are suggested to play a key role in increasing the displacement efficiency of oil. In previous studies, compositions of injected waterfloods (IJW) have been correlated to the observed oil recovery. This study highlights differences between IJW and ITW for different studies reported in literature.

**General information**

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Organisations: Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering, CERE – Center for Energy Resources Engineering, Technical University of Denmark
Authors: Chakravarty, K. H. (Intern), Fosbøl, P. L. (Intern), Thomsen, K. (Intern)
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High-Performance Small-Scale Solvers for Moving Horizon Estimation

In this paper we present a moving horizon estimation (MHE) formulation suitable to easily describe the quadratic programs (QPs) arising in constrained and nonlinear MHE. We propose algorithms for factorization and solution of the underlying Karush-Kuhn-Tucker (KKT) system, as well as the efficient implementation techniques focusing on small-scale problems. The proposed MHE solver is implemented using custom linear algebra routines and is compared against implementations using BLAS libraries. Additionally, the MHE solver is interfaced to a code generation tool for nonlinear model predictive control (NMPC) and nonlinear MHE (NMHE). On an example problem with 33 states, 6 inputs and 15 estimation intervals execution times below 500 microseconds are reported for the QP underlying the NMHE.

Importance of fines in smart water enhanced oil recovery (SmW-EOR) for chalk outcrops

In SmW-EOR it is generally believed that precipitation of brines must be avoided since it can have a negative impact on the SmW sweep efficiency. But substitution of Mg$^{2+}$ by Ca$^{2+}$ on calcite surfaces (a well-accepted phenomenon) can change the brine combination and enhance the possibility of fine formation at speciation. Considering this phenomenon we analyze the possibility of fines formation and its influence in SmW-EOR. To calculate the brine speciation and the amount of precipitate formed at different pressure and temperature conditions, we use the Extended UNIQUAC model for 61 SmW-EOR experiments reported in literature. Both the amount of available soluble SO$_4^{2-}$ (aq) in the solution and the amount of CaSO$_4$ precipitation has been calculated and correlated to the corresponding oil recovery.
SSF. Batch-SSF resulted in an ethanol yield of 75-76% and an ethanol concentration of 53 g/L. Prehydrolysis prior to batch SSF did not improve the ethanol yield compared with batch SSF. Fedbatch SSF, on the other hand, increased the yield, independent of the feeding conditions used (79-81%, 57-60 g/L). If the initial amount of solids during fed-batch SSF was lowered, the yield could be improved to some extent. When decreasing the enzyme dosage, the greatest decrease in yield was seen in the fed-batch mode (75%), while lower or the same yield was seen in batch mode with and without prehydrolysis (73%). This resulted in similar ethanol yields in all methods. However, the residence time to achieve the final ethanol yield was shorter using fed-batch. This shows that fed-batch can be a better alternative also at a lower enzyme loading.
Investigation of spore forming bacterial flooding for enhanced oil recovery in a North Sea chalk Reservoir

Little has been done to study microbial enhanced oil recovery (MEOR) in chalk reservoirs. The present study focuses on core flooding experiments designed to see microbial plugging and its effect on oil recovery. A pressure tapped core holder was used for this purpose. A spore forming bacteria Bacillus licheniformis 421 was used as it was shown to be a good candidate in a previous study. Bacterial spore can penetrate deeper into the chalk rock, squeezing through the pore throats. Our results showed that injection of B. licheniformis 421 as a tertiary oil recovery method, in the residual oil saturation state, was able to produce additionally 1.0-2.3% original oil in place (OOIP) in homogeneous cores and 6.9-8.8% OOIP in heterogeneous cores. In addition, the pressure gradient was much higher in the heterogeneous cores, which confirms that bacterial selective plugging plays an important role in higher oil production from the heterogeneous chalk rock. In all cases, an incubation period ('shut-in') after the bacterial and/or nutrient injection was needed to give sufficient time for the bacteria to grow inside the core and to produce more oil. Our findings show potential application of bacteria as a plugging agent in heterogeneous chalk cores to improve oil production.

General information
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Organisations: Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering, Maersk Oil and Gas A/S
Authors: Halim, A. Y. (Intern), Nielsen, S. M. (Intern), Eliasson Lantz, A. (Intern), Sander Suicmez, V. (Ekstern), Lindeloff, N. (Ekstern), Shapiro, A. (Intern)
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Web of Science (2015): Indexed yes
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Scopus rating (2014): SJR 0.692 SNIP 1.751 CiteScore 1.95
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Scopus rating (2013): SJR 0.822 SNIP 1.901 CiteScore 1.73
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BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.774 SNIP 1.666 CiteScore 1.42
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.648 SNIP 1.41 CiteScore 1.29
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
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Scopus rating (2010): SJR 0.746 SNIP 1.724
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Measurement of vapor-liquid-liquid phase equilibrium—Equipment and results

There exists a need for new accurate and reliable experimental data, preferably with full characterization of all the phases present in equilibrium. The need for high-quality experimental phase equilibrium data is the case for the chemical industry in general. All areas deal with processes whose optimization is dependent on phase equilibrium data. The objective of this work is to provide experimental data for hydrocarbon systems with polar chemicals such as alcohols, glycols and water. A new experimental equipment was designed and constructed for measurement of multi-phase equilibrium in hydrocarbon-water-gas hydrate inhibitor systems, at temperatures ranging from 283 to 353 K and at pressures up to 40 MPa. The core of the equipment is an equilibrium cell, equipped with sapphire windows and connected to an analytical system by capillary samplers. New vapor-liquid-liquid equilibrium data are reported for methane + n-hexane + methanol + water at 296.2 K and pressures of 6 to 10 MPa. The Cubic-Plus-Association (CPA) equation of state is used to model the phase equilibria data measured. A good agreement between predictions and experimental data is observed, supporting the reliability of the new experimental data. (C) 2015 Elsevier B.V. All rights reserved.
Modeling MEA with the CPA equation of state: A parameter estimation study adding local search to PSO algorithm

Due to the intensification of environmental constrains combined with the tendency to process crude oils with high C/H, S/H ratios and natural gas with increasing CO₂/CH₄ and H₂S/CH₄ ratios, acid gas removal from gas streams is probably the most required process in the petroleum and gas industries nowadays. Absorption with aqueous alkanolamines such as MEA, is one commonly used process for this purpose. On modeling MEA with CPA, it has been shown that only the co-
volume b parameter does not present local minima near the final solution and, also, VLE data are not sufficient to estimate reliable parameters for MEA. This work proposes adding LLE information systematically in the CPA parameter estimation procedure. At first, the parameter search space is defined by the results from the PSO sensitivity analysis for VLE considering the experimental error for vapor pressures and liquid densities (objective function cut off). Then, two possible methodologies are discussed: the first one uses all the possible parameter sets and check them against the LLE and VLE experimental data. The second method explicitly incorporates LLE information into the objective function and uses both PSO and PSO-simplex hybrid algorithm to improve the convergence and refine the final solution. With this methodology it was possible to model simultaneously LLE and VLE. The CPA was then applied for a mixture containing cross-association (MEA-water) and the results show good agreement with experimental data indicating the effectiveness of the proposed strategies.

**General information**

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**Organisations:** Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Ressources Engineering, Universidade Federal do Rio de Janeiro, Universidade Federal Fluminense  
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Web of Science (2015): Indexed yes  
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Scopus rating (2014): SJR 0.982 SNIP 1.248 CiteScore 2.28  
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Web of Science (2012): Indexed yes  
BFI (2011): BFI-level 2  
Scopus rating (2011): SJR 1.034 SNIP 1.234 CiteScore 2.26  
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Web of Science (2011): Indexed yes  
BFI (2010): BFI-level 2  
Scopus rating (2010): SJR 0.986 SNIP 1.317  
Web of Science (2010): Indexed yes  
BFI (2009): BFI-level 2  
Scopus rating (2009): SJR 1.133 SNIP 1.164  
Web of Science (2009): Indexed yes  
BFI (2008): BFI-level 1  
Scopus rating (2008): SJR 1.227 SNIP 1.09
Modeling of Dissolution Effects on Waterflooding

Physico-chemical interactions between the fluid and reservoir rock due to the presence of active components in the injected brine produce changes within the reservoir and can significantly impact the fluid flow. We have developed a 1D numerical model for waterflooding accounting for dissolution and precipitation of the components. Extending previous studies, we consider an arbitrary chemical non-equilibrium reaction-induced dissolution. We account for different individual volumes that a component has when precipitated or dissolved. This volume non-additivity also affects the pressure and the flow rate. An equation of state is used to account for brine density variation with regard to pressure and composition. We present a numerical study of the evolution of the reservoir parameters in the framework of the developed model. It is demonstrated that the systems characterized by large Damkohler numbers (fast reaction rates) may exhibit rapid increase of porosity and permeability near the inlet probably indicating a formation of high permeable channels (wormholes). Water saturation in the zone of dissolution increases due to an increase in the bulk volume accessible for the injected fluid. Volumetric non-additivity is found to be responsible for insignificant change in the velocity of the displacement front.

General information
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Organisations: Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Ressources Engineering
Authors: Alexeev, A. (Intern), Shapiro, A. (Intern), Thomsen, K. (Intern)
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Journal: Transport in Porous Media
Volume: 106
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Modeling phase equilibria for acid gas mixtures using the CPA equation of state. Part IV. Applications to mixtures of CO$_2$ with alkanes

The thermodynamic properties of pure gaseous, liquid or supercritical CO$_2$ and CO$_2$ mixtures with hydrocarbons and other compounds such as water, alcohols, and glycols are very important in many processes in the oil and gas industry. Design of such processes requires use of accurate thermodynamic models, capable of predicting the complex phase behavior of multicomponent mixtures as well as their volumetric properties. In this direction, over the last several years, the cubic-plus-association (CPA) thermodynamic model has been successfully used for describing volumetric properties and phase behavior of several mixtures of interest in oil and gas industry. The purpose of this work is to evaluate the performance of CPA for CO$_2$-alkane mixtures. CPA calculations were performed using different association schemes for CO$_2$. Firstly, CO$_2$ was treated as non-associating fluid and, at a second level, CO$_2$ was treated as self-associating fluid,
using the 2B, 3B and 4C association schemes. A systematic investigation of the CPA performance in correlating the phase behavior of CO$_2$-alkane mixtures has been performed. Mixtures with alkanes up to n-hexatriacontane (n-C$_{36}$) were investigated and the corresponding binary interaction parameters were estimated with all modeling approaches for CO$_2$. CPA parameters were previously available for alkanes up to n-eicosane (n-C$_{20}$) and new parameters have been estimated for heavier alkanes based on DIPPR correlations. CPA correlations were compared with literature experimental data for three heavy alkanes and a satisfactory agreement was observed. The CPA performance is discussed including trends of the interaction parameters with chain length and comparison to literature studies.

**General information**

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Organisations: CERE – Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering, Aristotle University of Thessaloniki
Authors: Tsivintzelis, I. (Intern), Ali, S. (Intern), Kontogeorgis, G. (Intern)
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- Scopus rating (2015): SJR 0.874 SNIP 0.998 CiteScore 1.99
- Web of Science (2015): Indexed yes
- BFI (2014): BFI-level 2
- Scopus rating (2014): SJR 0.982 SNIP 1.248 CiteScore 2.28
- Web of Science (2014): Indexed yes
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- Scopus rating (2013): SJR 1.007 SNIP 1.274 CiteScore 2.31
- ISI indexed (2013): ISI indexed yes
- Web of Science (2013): Indexed yes
- BFI (2012): BFI-level 2
- Scopus rating (2012): SJR 1.152 SNIP 1.286 CiteScore 2.31
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- ISI indexed (2011): ISI indexed yes
- Web of Science (2011): Indexed yes
- BFI (2010): BFI-level 2
- Scopus rating (2010): SJR 0.986 SNIP 1.317
- Web of Science (2010): Indexed yes
- BFI (2009): BFI-level 2
- Scopus rating (2009): SJR 1.133 SNIP 1.164
- Web of Science (2009): Indexed yes
- BFI (2008): BFI-level 1
- Scopus rating (2008): SJR 1.227 SNIP 1.09
- Web of Science (2008): Indexed yes
- Scopus rating (2007): SJR 1.031 SNIP 1.151
Modeling the binary system Mn(NO$_3$)$_2$-H$_2$O with the extended universal quasichemical (UNIQUAC) model

In this study, new experimental data for the binary system of Mn(NO$_3$)$_2$-H$_2$O are presented in the temperature range from -29°C to 35°C at atmospheric pressure using the conductometric method. This synthetic method is an accurate experimental procedure in the determination of the solubility of salts in aqueous solutions. Thermodynamic modeling for the binary system of Mn(NO$_3$)$_2$-H$_2$O is also presented based on this new experimental solubility data and some modification on the available data bank. Model parameters for this system were determined and revisited; these parameters are generally valid in the entire range of temperature and composition of the salt.

General information

State: Published
Organisations: Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering, University Hassan I
Authors: Arrad, M. (Ekstern), Kaddami, M. (Ekstern), Maous, J. (Ekstern), Thomsen, K. (Intern)
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Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.874 SNIP 0.998 CiteScore 1.99
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 0.982 SNIP 1.248 CiteScore 2.28
Modeling the liquid-liquid equilibrium of petroleum fluid and polar compounds containing systems with the PC-SAFT equation of state

A critical test for the perturbed-chain statistical associating fluid theory (PC-SAFT) equation of state (FOS) is the modeling of systems containing petroleum fluid and polar compounds. In this work, two approaches are proposed for the simplified PC-SAFT EOS to obtain the necessary pure component parameters for the characterized non-associating pseudo-components of petroleum fluids. New pure component parameters of mono-ethylene glycol (MEG) are obtained by considering the liquid liquid equilibrium (LLE) data of MEG with normal hydrocarbons in the estimation process and a simple binary interaction scheme of MEG with pseudo-components is proposed. These new parameters are applied to model LLE of the systems of petroleum fluid + MEG with or without water. The results show that the simplified PC-SAFT EOS yields promising predictions of the key mutual solubility of these systems: 15-18% overall deviations for the systems.
of petroleum fluid + MEG and 23-25% overall deviations for the systems of petroleum fluid + MEG + water. The two approaches are further studied in a more theoretical manner to show the relationship between the solubility of petroleum fluid in the polar phase and the PC-SAFT parameter segment diameter. (C) 2015 Elsevier B.V. All rights reserved.

**General information**

*State:* Published

*Organisations:* Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering, Department of Chemistry

*Authors:* Liang, X. (Intern), Yan, W. (Intern), Thomsen, K. (Intern), Kontogeorgis, G. M. (Intern)

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- ISI indexed (2013): ISI indexed yes
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- Web of Science (2012): Indexed yes
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- Scopus rating (2011): SJR 1.034 SNIP 1.234 CiteScore 2.26
- ISI indexed (2011): ISI indexed yes
- Web of Science (2011): Indexed yes
- BFI (2010): BFI-level 2
- Scopus rating (2010): SJR 0.986 SNIP 1.317
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- Scopus rating (2009): SJR 1.133 SNIP 1.164
- Web of Science (2009): Indexed yes
- BFI (2008): BFI-level 1
- Scopus rating (2008): SJR 1.227 SNIP 1.09
- Web of Science (2008): Indexed yes
- Scopus rating (2007): SJR 1.031 SNIP 1.151
- Web of Science (2007): Indexed yes
- Scopus rating (2006): SJR 1.034 SNIP 1.245
- Web of Science (2006): Indexed yes
- Scopus rating (2005): SJR 1.009 SNIP 1.3
Modeling Water Saturation Points in Natural Gas Streams Containing CO₂ and H₂S-Comparisons with Different Equations of State

Since the discovery of the Pre-Salt layer in Brazilian waters, production of high gas-oil ratio (GOR) has increased considerably. This gas has a high content of water, CO₂, and sometimes H₂S. A study in different conditions was conducted using several equations of state (EoS) such as Peng-Robinson, GERG-modified Peng-Robinson (PR-ISO-04), Soave-Redlich-Kwong, and Cubic Plus Association (CPA). Petrobras Process Simulator has been used to perform the phase equilibrium calculations. All the EoS except for CPA used parameters from the literature. A new parameter estimation procedure for CPA has been proposed using a particle swarm optimization algorithm followed by the SIMPLEX method presenting themselves together as an optimal approach. The results show that PR-ISO-04 can be considered to be an improvement compared to the original Peng-Robinson but CPA appears to be the most promising approach to be used for predicting dew points for water-containing mixtures, especially at high pressures.
Modelling phase equilibria for acid gas mixtures using the CPA equation of state. Part V: Multicomponent mixtures containing CO₂ and alcohols

The Cubic plus association (CPA) equation of state has been previously applied to a variety of binary systems containing CO₂ with alkanes, water, alcohols and glycols as well as a few multicomponent mixtures (with triethylene glycol, water and methane). In this study, we evaluate the performance of CPA for ternary and multicomponent CO₂ mixtures containing alcohols (methanol, ethanol or propanol) water and hydrocarbons. This work belongs to a series of studies aiming to arrive in a single "engineering approach" for applying CPA to acid gas mixtures, without introducing significant changes to the model. In this direction, CPA results were obtained using various approaches, i.e. different association schemes for pure
CO₂ (assuming that it is a non-associating compound, or that it is a self-associating fluid with two, three or four association sites) and different possibilities for modelling mixtures of CO₂ with water and alcohols (only use of one interaction parameter k_ij or assuming cross-association interactions and obtaining the relevant parameters either via a combining rule or using an experimental value for the cross-association energy). It is concluded that CPA is a powerful model that can be used for predictions of multicomponent mixture properties using no adjustable parameters fitted to the multicomponent system data. The results are satisfactory and rather similar with most investigated approaches. However, an overall assessment, also based on the obtained results of this series of studies [Tsivintzelis et al. Fluid Phase Equilib. 306 (2011) 38-56, J. Chem. Eng. Data 59 (2014) 2955-2972, Fluid Phase Equilib. 397 (2015) 1-17], reveals that the best approaches are those where the cross-association (solvation) of CO₂ with alcohols and water is explicitly accounted for or alternatively when CO₂ is considered to be a self-associating molecule (with three or four sites). Furthermore, it is recommended to use the experimental values of the cross-association energy for CO₂-water and CO₂-alcohols.

General information
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Scopus rating (2016): CiteScore 3.01 SJR 0.976 SNIP 1.266
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BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.921 SNIP 1.216 CiteScore 2.71
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.139 SNIP 1.461 CiteScore 2.89
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.097 SNIP 1.503 CiteScore 3.18
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.329 SNIP 1.669 CiteScore 3.38
ISI indexed (2012): ISI indexed yes
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BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.055 SNIP 1.483 CiteScore 3.03
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.337 SNIP 1.571
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.288 SNIP 1.431
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.231 SNIP 1.496
Model predictive control for wind power gradients

We consider the operation of a wind turbine and a connected local battery or other electrical storage device, taking into account varying wind speed, with the goal of maximizing the total energy generated while respecting limits on the time derivative (gradient) of power delivered to the grid. We use the turbine inertia as an additional energy storage device, by varying its speed over time, and coordinate the flows of energy to achieve the goal. The control variables are turbine pitch, generator torque and charge/discharge rates for the storage device, each of which can be varied over given ranges. The system dynamics are quite non-linear, and the constraints and objectives are not convex functions of the control inputs, so the resulting optimal control problem is difficult to solve globally. In this paper, we show that by a novel change of variables, which focuses on power flows, we can transform the problem to one with linear dynamics and convex constraints. Thus, the problem can be globally solved, using robust, fast solvers tailored for embedded control applications. We implement the optimal control problem in a receding horizon manner and provide extensive closed-loop tests with real wind data and modern wind forecasting methods. The simulation results using real wind data demonstrate the ability to reject the disturbances from fast changes in wind speed, ensuring certain power gradients, with an insignificant loss in energy production.

General information
State: Published
Organisations: Center for Energy Resources Engineering, Department of Applied Mathematics and Computer Science, Scientific Computing, Vestas Technology R&D, Stanford University
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MPC Related Computational Capabilities of ARMv7A Processors

In recent years, the mass market of mobile devices has pushed the demand for increasingly fast but cheap processors. ARM, the world leader in this sector, has developed the Cortex-A series of processors with focus on computationally intensive applications. If properly programmed, these processors are powerful enough to solve the complex optimization problems arising in MPC in real-time, while keeping the traditional low-cost and low-power consumption. This makes these processors ideal candidates for use in embedded MPC. In this paper, we investigate the floating-point capabilities of Cortex A7, A9 and A15 and show how to exploit the unique features of each processor to obtain the best performance, in the context of a novel implementation method for the linear-algebra routines used in MPC solvers. This method adapts high-performance computing techniques to the needs of embedded MPC. In particular, we investigate the performance of matrix-matrix and matrix-vector multiplications, which are the backbones of second- and first-order methods for convex optimization. Finally, we test the performance of MPC solvers implemented using these optimized linear-algebra routines.
Multicomponent Adsorption Model for Polar and Associating Mixtures

The multicomponent potential adsorption theory (MPTA) is revisited in this work for polar and associating systems. MPTA is used in combination with the CPA equation of state. Previous Studies have shown that both MPTA and other theories present difficulties for complex systems. Some of these problems could be due to the fact that the original MPTA assumes that a given adsorbent has the same adsorption capacity (for example, porous volume) for all the adsorbed substances and is adjusted simultaneously to many data. This is a simplified picture, as experimental data indicate that the adsorption capacities of the various components may also differ. In this paper we develop a scheme for the distribution of the potential, which accounts for the presence of the porous space occupied either by just one component or by both components. These capacities are determined by adjustment of the potentials to experimental data on single-component adsorption. We show that MPTA involving the different adsorption capacities for the different components is capable of predicting binary adsorption data for most of the mixtures considered. In our application of MPTA, we used both the well-known Dubinin-Radushkevich-Astakhov potentials and the potentials directly restored from experimental data by solving the inverse problem. Application of the latter potentials clearly demonstrates the importance of the difference in adsorption capacities. However, the quality of prediction of binary adsorption is similar for both potentials. Thus, we feel that there is no need to use more complex potentials provided that the difference in the individual adsorption capacities is accounted for.
For a sound field observed on a sensor array, compressive sensing (CS) reconstructs the direction of arrival (DOA) of multiple sources using a sparsity constraint. The DOA estimation is posed as an underdetermined problem by expressing the acoustic pressure at each sensor as a phase-lagged superposition of source amplitudes at all hypothetical DOAs. Regularizing with an ℓ1-norm constraint renders the problem solvable with convex optimization, and promoting sparsity gives high-resolution DOA maps. Here the sparse source distribution is derived using maximum a posteriori estimates for both single and multiple snapshots. CS does not require inversion of the data covariance matrix and thus works well even
for a single snapshot where it gives higher resolution than conventional beamforming. For multiple snapshots, CS outperforms conventional high-resolution methods even with coherent arrivals and at low signal-to-noise ratio. The superior resolution of CS is demonstrated with vertical array data from the SWellEx96 experiment for coherent multi-paths.

**General information**

State: Published
Organisations: Center for Energy Resources Engineering, Department of Applied Mathematics and Computer Science, Scientific Computing, Acoustic Technology, Technische Universität Wien, University of California, San Diego
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Scopus rating (2012): SJR 0.763 SNIP 1.622 CiteScore 1.75
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Scopus rating (2010): SJR 0.754 SNIP 1.528
Web of Science (2010): Indexed yes
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Scopus rating (2009): SJR 0.783 SNIP 1.717
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 0.848 SNIP 1.633
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 0.865 SNIP 1.647
Web of Science (2007): Indexed yes
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Multiple snapshot compressive beamforming

For sound fields observed on an array, compressive sensing (CS) reconstructs the multiple source signals at unknown directions-of-arrival (DOAs) using a sparsity constraint. The DOA estimation is posed as an underdetermined problem expressing the field at each sensor as a phase-lagged superposition of source amplitudes at all hypothetical DOAs. CS is applicable even for a single observation snapshot achieving a higher resolution than conventional beamforming. For multiple snapshots, CS outperforms conventional high-resolution methods, even with coherent arrivals and at low signal-to-noise ratio.

Natural gas hydrate formation and inhibition in gas/crude oil/aqueous systems

Gas hydrate formation in multi phase mixtures containing an aqueous phase (with dissolved salts), reservoir fluid (crude oil) and natural gas phase was investigated by using a standard rocking cell (RC-5) apparatus. The hydrate formation temperature was reduced in the presence of crude oils in comparison with that in pure water. This observed hydrate inhibition potential shows significant variation depending on the type of crude oil. The influence of crude oil composition (saturates, aromatics, resins and asphaltenes) on this behavior was probably due to the existence of a combination of different inhibition mechanisms and potentially a competition among inhibition-promotion mechanisms. Moreover, the hydrate formation time has been determined at different water cuts in each crude oil and it was found that the inhibition capability increases with an increase in the oil content. The effect of the biodegradable commercial kinetic inhibitor (Luvicap-Bio) on natural gas hydrate formation with and without crude oil (30%) was investigated. The strength of kinetic inhibitor was not affected by salts, but decreased significantly in the presence of crude oil. Data for hydrate formation at practical conditions can contribute to the safe operation of sub sea pipelines in the oil and gas industry.
New Variant of the Universal Constants in the Perturbed Chain-Statistical Associating Fluid Theory Equation of State

The Perturbed Chain-Statistical Associating Fluid Theory Equation of State (PC-SAFT EOS) has been successfully applied to model phase behavior of various types of systems, while it is also well-known that the PC-SAFT EOS has difficulties in describing some second-order derivative properties. In this work, the temperature and volume dependencies of the PC-SAFT EOS have been analyzed based on the total reduced residual Helmholtz free energy from the well-established reference equations. The ranges of parameters and temperature, in which the original PC-SAFT EOS give zero or more than three volume roots, have been analyzed. Then, a practical procedure has been proposed to refit the universal constants of the PC-SAFT EOS with the purpose of fixing the numerical pitfalls in the real application ranges and reusing the original parameters. It is shown that the new universal constants have practically resolved the mostly criticized numerical pitfall, that is, the presence of more than three volume roots at real application conditions. Finally, the possibility of using the original PC-SAFT EOS parameters with the new universal constants has been investigated for the phase equilibria of the systems containing hydrocarbons, chemicals, water, or polymers.

General information

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Organisations: Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering
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Web of Science (2015): Indexed yes
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Scopus rating (2014): SJR 1.012 SNIP 1.292 CiteScore 2.85
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Web of Science (2013): Indexed yes
Oil and gas pipelines with hydrophobic surfaces better equipped to deal with gas hydrate flow assurance issues

Gas hydrate deposition can cause plugging in oil and gas pipelines with resultant flow assurance challenges. Presently, the energy industry uses chemical additives in order to manage hydrate formation, however these chemicals are expensive and may be associated with safety and environmental concerns. Here we show the effect of a hydrophobically coated surface on hydrate formation in the presence of an antifreeze protein type I (AFP I) and a biodegradable synthetic polymer (LuvicapBio) in a high pressure crystallizer setup. The hydrophobic surface increased the hydrate induction time and reduced the hydrate growth significantly in pure deionized water (control). Furthermore, in the presence of 0.02 wt% of LuvicapBio or 0.014 wt% AFP I in the hydrophobic coated crystallizer; the hydrate growth was reduced to almost the same level as obtained with 0.20 wt% of LuvicapBio in a stainless steel crystallizer. This indicates that 10 to 14 times less KHI is needed in the presence of a hydrophobically coated surface. These experimental studies suggest that the use of hydrophobic surfaces or pipelines could serve as an alternative or additional flow assurance approach for gas hydration mitigation and management.
On the viscosity of two 1-butyl-1-methylpyrrolidinium ionic liquids: effect of the temperature and pressure

A new calibration procedure was used and four new temperature probes have been placed on a falling-body viscometer to improve its accuracy. The new configuration and calibration procedure allow measuring viscosities with an uncertainty of 3.5% at pressures up to 150 MPa. This device was employed to measure viscosities as a function of temperature and pressure for two ionic liquids (ILs): 1-butyl-1-methylpyrrolidinium tris(pentafluoroethyl)trifluorophosphate and 1-butyl-1-methylpyrrolidinium trifluoromethanesulfonate. Besides, we have measured the flow curves at pressures up to 75 MPa and shear rates up to 1000 s⁻¹ in a Couette rheometer. Dynamic viscosities were correlated as a function of temperature and pressure with four different equations with average absolute deviation lower than 1%. The pressure-viscosity and temperature-viscosity derived properties were analyzed and compared with those of other ionic liquids. Furthermore, experimental data were used to check the application of the thermodynamic scaling approach as well as the hard-sphere scheme. Both models represent the viscosity values with average relative deviations lower than 2%.

General information
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Ionic liquid, Viscosity, High Pressure, Thermodynamic Scaling, Hard Spheres Scheme
Optimization of Spore Forming Bacteria Flooding for Enhanced Oil Recovery in North Sea Chalk Reservoir
Little has been done to study microbial enhanced oil recovery (MEOR) in chalk reservoirs. The present study focused on core flooding experiments to see microbial plugging and its effect on oil recovery. A pressure tapped core holder with pressure ports at 1.2 cm, 3.8 cm, and 6.3 cm from the inlet was used for this purpose. A spore forming bacterium, *Bacillus licheniformis* 421, was used as it was shown to be a good candidate in the previous study. Bacterial spore can penetrate deeper into the chalk rock, squeezing through the pore throats. Our results show that *B. licheniformis* 421 when injected as a secondary technique can recover 4% more of the original oil in place (OOIP) as compared with the seawater flooding. Furthermore, when applied as tertiary technique it can recover 1.4% OOIP of the residual oil. The effective permeability decreased in the first two sections of the core (0-1.2 cm and 1.2-3.8 cm) during bacteria injection. Further seawater flooding after three days shut in period showed that permeability gradually increased in the first two sections of the core and started to decrease in the third section of the core (3.8-6.3 cm). Complete plugging was never observed in our experiments.

Permeability in Rotliegend gas sandstones to gas and brine as predicted from NMR, mercury injection and image analysis
Permeability characterisation of low permeability, clay-rich gas sandstones is part of production forecasting and reservoir management. The physically based Kozeny (1927) equation linking permeability with porosity and pore size is derived for a porous medium with a homogeneous pore size, whereas the pore sizes in tight sandstones can range from nm to μm. Nuclear magnetic resonance (NMR) transverse relaxation was used to estimate a pore size distribution for 63 samples of Rotliegend sandstone. The surface relaxation parameter required to relate NMR to pore size is estimated by combination of NMR and mercury injection data. To estimate which pores control permeability to gas, gas permeability was calculated for each pore size increment by using the Kozeny equation. Permeability to brine is modelled by assuming a bound water layer on the mineral pore interface. The measured brine permeabilities are lower than predicted based on bound water alone for these illite rich samples. Based on the fibrous textures of illite as visible in electron microscopy we speculate that these may contribute to a lower brine permeability.
Phase Envelope Calculations for Reservoir Fluids in the Presence of Capillary Pressure

Reservoir fluids are multicomponent mixtures in confined spaces, where the role of capillary force becomes important when the average pore size is on the order of tens of nanometers, such as in tight rocks and shale. We present an algorithm for calculating the phase envelope of multicomponent mixtures in the presence of capillary pressure. The algorithm uses a rigorous equation of state (EoS) model, such as the Soave-Redlich-Kwong EoS, for phase equilibrium, and the Young-Laplace equation for the capillary pressure. The interfacial tension is calculated using a parachor based model. A full Newton method is employed to solve the governing equations of the vapor-liquid equilibria coupled with the capillary pressure equation. For a stable and automatic construction of the phase envelope sensitivity analysis is used in each step. The developed algorithm can reliably generate not just the bubble and dew point curves but also other quality lines with vapor fractions between 0 and 1. The algorithm has been used to calculate the phase envelopes of binary, multicomponent and reservoir fluid systems for pore radius from 10 to 50 nm. The presence of capillary pressure changes the saturation pressures in the whole phase envelope except at the critical point. The bubble point curve shows a negative change while the dew point curve shows positive and negative changes in the upper dew point branch and the lower dew point branch, respectively. In particular, the cricondentherm is also shifted towards a higher temperature. The change in the phase envelope becomes larger as the pore size decreases. The effects of composition and gas oil ratios are also discussed.

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Organisations: Center for Energy Resources Engineering, Department of Chemistry, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Ressources Engineering
Pressure dependence of the solubility of light fullerenes in 1-hexanol from 298.15 K to 363.15 K

The solubility of light fullerenes ($\text{C}_{60}$ and $\text{C}_{70}$) in 1-hexanol was investigated in the range of pressures of 0.1-100 MPa and in the range of temperatures of 298.15-363.15 K. In all of the studied temperatures, solubility increases monotonously with increasing pressure. At ambient pressure, we have found that the temperature dependence of solubility in the binary system $\text{C}_{60}$-1-hexanol is non-monotonic: the solubility diagram consists of two branches corresponding to the crystallization of different solid phases and one invariant point corresponding to the simultaneous saturation of both phases (monosolvated fullerene $\text{C}_{60}$ and non-solvated $\text{C}_{60}$). The composition of the solid crystallosolvate was determined by thermogravimetric analysis. The solubility diagram of the binary system $\text{C}_{70}$-1-hexanol in the temperature range of 298.15-328.15 K at 0.1 MPa consists of only one branch corresponding to the crystallization of non-solvated $\text{C}_{70}$. 

General information

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Web of Science (2015): Indexed yes
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Scopus rating (2014): SJR 0.637 SNIP 1.126 CiteScore 2.34
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.611 SNIP 1.082 CiteScore 2.07
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Web of Science (2013): Indexed yes
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Scopus rating (2012): SJR 0.673 SNIP 1.041 CiteScore 1.62
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Profiling of Indigenous Microbial Community Dynamics and Metabolic Activity During Enrichment in Molasses-Supplemented Crude Oil-Brine Mixtures for Improved Understanding of Microbial Enhanced Oil Recovery

Anaerobic incubations using crude oil and brine from a North Sea reservoir were conducted to gain increased understanding of indigenous microbial community development, metabolite production, and the effects on the oil–brine system after addition of a complex carbon source, molasses, with or without nitrate to boost microbial growth. Growth of the indigenous microbes was stimulated by addition of molasses. Pyrosequencing showed that specifically *Anaerobiculum*, *Petrotoga*, and *Methanothermococcus* were enriched. Addition of nitrate favored the growth of *Petrotoga* over *Anaerobiculum*. The microbial growth caused changes in the crude oil–brine system: formation of oil emulsions, and reduction of interfacial tension (IFT). Reduction in IFT was associated with microbes being present at the oil–brine interphase. These findings suggest that stimulation of indigenous microbial growth by addition of molasses has potential as microbial enhanced oil recovery (MEOR) strategy in North Sea oil reservoirs.
Profit and Risk Measures in Oil Production Optimization

In oil production optimization, we usually aim to maximize a deterministic scalar performance index such as the profit over the expected reservoir lifespan. However, when uncertainty in the parameters is considered, the profit results in a random variable that can assume a range of values depending on the value of the uncertain parameters. In this case, a problem reformulation is needed to properly define the optimization problem. In this paper we describe the concept of risk and we explore how to handle the risk by using appropriate risk measures. We provide a review on various risk measures reporting pro and cons for each of them. Finally, among the presented risk measures, we identify two of them as appropriate risk measures when minimizing the risk.

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PVT modeling of reservoir fluids using PC-SAFT EoS and Soave-BWR EoS

Cubic equations of state, such as the Soave-Redlich-Kwong (SRK) and the Peng-Robinson (PR) EoS, are still the mostly used models in PVT modeling of reservoir fluids, and almost the exclusively used models in compositional reservoir simulations. Nevertheless, it is promising that recently developed non-cubic EoS models, such as the Perturbed Chain Statistical Associating Fluid Theory (PC-SAFT) EoS and the Soave modified Benedict-Webb-Rubin (Soave-BWR) EoS, may partly replace the roles of these classical cubic models in the upstream oil industry. Here, we attempt to make a comparative study of non-cubic models (PC-SAFT and Soave-BWR) and cubic models (SRK and PR) in several important aspects related to PVT modeling of reservoir fluids, including density description for typical pure components in reservoir fluids, description of binary VLE, prediction of multicomponent phase envelopes, and PVT calculation of reservoir fluids. Extensive data are used in the comparison and the four models are treated as equally as possible. We adopt the method of Pedersen et al. as the framework for heptanes plus characterization and the same correlations for estimating the critical properties for SRK, PR and Soave-BWR. For PC-SAFT, new correlations for estimating its model parameters in heptanes plus are developed. The results reveal that the non-cubic models are clearly advantageous in density calculation of pure components. For binary VLE and multicomponent phase envelopes, the results are similar for the four models. For PVT prediction, the non-cubic models show advantages in some high pressure high temperature (HPHT) fluids but no clear advantages in general, indicating the necessity for further improvement of the characterization procedure.

General information
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Organisations: Center for Energy Resources Engineering, Department of Chemistry, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering
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Journal: Fluid Phase Equilibria
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Quantification of the recovered oil and water fractions during water flooding laboratory experiments

During core flooding experiments where water is injected in residual oil saturated core plugs, the fluids are often produced in small amounts. Oil and water come out of the core and are collected in glass vials using a fraction collector. Quantification of these fluids is often difficult since the volume might be less than a few microliters. In this study, we approach the determination of the oil volumes in flooding effluents using predetermined amounts of the North Sea oil with synthetic seawater. The UV/visible spectroscopy method and low-field NMR spectrometry are compared for this determination, and an account of advantages and disadvantages of each method is given. Both methods are reproducible with high accuracy. The NMR method was capable of direct quantification of both oil and water fractions, while the UV/visible spectroscopy quantifies only the oil fraction using a standard curve.

General information
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Organisations: Department of Civil Engineering, Section for Geotechnics and Geology, Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Ressources Engineering
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Real-time nonlinear MPC and MHE for a large-scale mechatronic application

Progress in optimization algorithms and in computational hardware made deployment of Nonlinear Model Predictive Control (NMPC) and Moving Horizon Estimation (MHE) possible to mechatronic applications. This paper aims to assess the computational performance of NMPC and MHE for rotational start-up of Airborne Wind Energy systems. The capabilities offered by an automatic code generation tool are experimentally verified on a real physical system, using a model comprising 27 states and 4 inputs at a sampling frequency of 25 Hz. The results show the feedback times less than 5 ms for the NMPC with more than 1500 variables.

General information
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Organisations: Department of Applied Mathematics and Computer Science, Scientific Computing, Center for Energy Resources Engineering, Chalmers University of Technology, KU Leuven
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Risk Associated With The Decompression Of High Pressure High Temperature Fluids - Study On Black Oil

Fluids produced from deep underground reservoirs may result in exponential increase in temperature. It is a consequence of adiabatic fluid decompression from the inverse Joule Thomson Effect (JTE). The phenomenon requires analysis in order to avoid any operational risks. This study evaluates the JTE upon decompression of black oil in high pressure-high temperature reservoirs. Also the effect caused by the presence of water and brine on the black oil is studied. The final temperature is calculated from the corresponding energy balance at isenthalpic and non-isenthalpic conditions. It is found that the final temperature of black oil increases upon adiabatic decompression. In the case of the isenthalpic process at initial conditions of the reservoir, e.g. 150°C and 1000 bars, it is found that the final temperature can increase to 173.7°C. At non-isenthalpic conditions the final temperature increases as well, but the increase is less. The effect of water is studied at different water fractions; it results in lower increase of the final temperature than observed for black oil. The presence of brine in black oil is also studied at different brine fractions. The addition of brine increases the final temperature but the increase is less than for pure black oil. Therefore, the presence of water and brine in black oil diminishes the heating effect.
observed initially for black oil.

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Organisations: Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering
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Solubility of hydrogen sulfide in aqueous solutions of N-methyldiethanolamine at high pressures
A static-analytic method was used to measure the H2S solubility in 50 wt% MDEA and in presence of methane as a makeup gas. The solubility was measured at 7000 kPa total pressure, and at 50 and 70 degrees C, for H2S partial pressures from 31 to 974 kPa. Measurements were also performed at 1500 kPa total pressure and 50 degrees C for H2S partial pressure span of 53-386 kPa. The measured data were compared to predictions using the Extended UNIQUAC model. The experimental data showed that the total pressure has a significant effect on H2S solubility in aqueous MDEA. The observed effect is shown to be dominated by the non-ideality of the gas, and it could be predicted by the pressure effect on the fugacity coefficient of H2S in the gas phase. The experimental data from this work are compared and shown to be consistent with earlier published data.
Sparse acoustic imaging with a spherical array

In recent years, a number of methods for sound source localization and sound field reconstruction with spherical microphone arrays have been proposed. These arrays have properties that are potentially very useful, e.g. omnidirectionality, robustness, compensable scattering, etc. This paper proposes a plane wave expansion method based on measurements with a spherical microphone array, and solved in the framework provided by Compressed Sensing. The proposed methodology results in a sparse solution, i.e. few non-zero coefficients, and it is suitable for both source localization and sound field reconstruction. In general it provides fine spatial resolution for localization (delta-like functions), and robust reconstruction (the noisy components are naturally suppressed). The validity and performance of the proposed method is examined, and its limitations as well as the underlying assumptions are addressed.

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Sparse DOA estimation with polynomial rooting

Direction-of-arrival (DOA) estimation involves the localization of a few sources from a limited number of observations on an array of sensors. Thus, DOA estimation can be formulated as a sparse signal reconstruction problem and solved efficiently with compressive sensing (CS) to achieve high-resolution imaging. Utilizing the dual optimal variables of the CS optimization problem, it is shown with Monte Carlo simulations that the DOAs are accurately reconstructed through polynomial rooting (Root-CS). Polynomial rooting is known to improve the resolution in several other DOA estimation methods. However, traditional methods involve the estimation of the cross-spectral matrix hence they require many snapshots and stationary incoherent sources and are suitable only for uniform linear arrays (ULA). Root-CS does not have these limitations as demonstrated on experimental towed array data from ocean acoustic measurements.

Study of wettability of calcite surfaces using oil-brine-enzyme systems for enhanced oil recovery applications

Enzymes have recently been considered as possible agents for enhanced oil recovery (EOR) acting at the liquid-solid interface. One way to assess this is via measuring the wettability of calcite surfaces, important for EOR methods in carbonaceous reservoirs. In the present work, we have experimentally investigated the effect of enzymes on the wettability of calcite mineral surfaces with oil-brine systems. The action of various enzymes, including esterases/lipases, carboxylases, proteases and oxidoreductases (along with two commercial mixtures) was studied by contact angle measurements and adhesion behaviour tests. Comparative studies with a surfactant, protein, purified enzyme, enzyme stabiliser using n-decane (as a model for the oil) have also been carried out in order to verify experimental results. The enzymes that have the highest effect on the wettability have been identified. Those enzymes, which were found the most promising from a practical perspective, have shown the ability to fully detach oil from the surface, even at very low enzyme concentrations. For example, esterases/lipases were found to strongly affect the wettability and to remove adhesion at concentrations as low as 0.1% of the enzyme product (corresponding to 0.002-0.005% protein). Likewise, proteases could also improve wettability, although the effect was not consistent and was dependent on impurities. Other enzymes had no effect on the wettability of calcite at the concentration studied. The main mechanism of enzymatic action has been found to be replacement of oil at the solid surface by the enzyme. Other mechanisms (modification of the surface tension or catalytic modification of hydrocarbons resulting in reducing the oil viscosity) have shown to be much less pronounced from the measurements reported here.
Techniques for hot embossing microstructures on liquid silicone rubbers with fillers

Embossing is an established process for the thermoplastic elastomers but not yet for the thermosetting elastomers. It has already been shown that hot embossing is a viable technology for imprinting microstructures in addition to curing thin silicone films at their gel point. It is one of the simplest, most cost-effective, and time-saving methods for replicating microstructures. In the present study, films made from liquid silicone rubber (LSR) formulations containing fillers are hot embossed under modified operating conditions. The use of such relatively hard silicone elastomers shows the versatility of this method that has been established for softer silicone elastomers. Also, as a proof of concept, a microstructured metal (nickel (Ni)) plate is used as an embosser for the films successfully. The ideal condition for hot embossing the LSR formulation (XLR 630 with titanium dioxide fillers) with a Ni embosser is 110°C preheating for 15–35 s, embossed with 2 bar pressure, and postheating for complete curing at 110°C for 3 min showing that the process is extremely fast.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, The Danish Polymer Centre, Center for Energy Resources Engineering
Authors: Vudayagiri, S. (Intern), Yu, L. (Intern), Skov, A. L. (Intern)
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BFI (2018): BFI-level 1
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Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 0.278 SNIP 0.533 CiteScore 0.76
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.243 SNIP 0.481 CiteScore 0.61
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.208 SNIP 0.471 CiteScore 0.6
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.404 SNIP 0.592 CiteScore 0.75
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.307 SNIP 0.782 CiteScore 0.75
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Testing antifreeze protein from the longhorn beetle *Rhagium mordax* as a kinetic gas hydrate inhibitor using a high-pressure micro differential scanning calorimeter

Low dosage kinetic hydrate inhibitors are employed as alternatives to expensive thermodynamic inhibitors to manage the risk of hydrate formation inside oil and gas pipelines. These chemicals need to be tested at appropriate conditions in the laboratory before deployment in the field. A high pressure micro differential scanning calorimeter HP-mu DSC VII (Setaram Inc.) containing two 50 cc high pressure cells (maximum operating pressure 40 MPa; temperature range -40 to 120 degrees C) was employed to observe methane hydrate formation and decomposition in the presence of hyperactive antifreeze protein from *Rhagium mordax* (RmAFP) and biodegradable synthetic kinetic inhibitor Luvicap Bio. A systematic capillary dispersion method was used, and this method enhanced the ability to detect the effect of various inhibitors on hydrate formation with small quantities. The presence of RmAFP and Luvicap Bio influence (inhibit) the hydrate formation phenomena significantly. Luvicap Bio (relative strength compared to buffer: 13.3 degrees C) is stronger than RmAFP (9.8 degrees C) as a nucleation inhibitor. However, the presence RmAFP not only delays hydrate nucleation but also reduces the amount of hydrate formed (20%-30%) after nucleation significantly. Unlike RmAFP, Luvicap Bio promoted the amount of hydrate formed after nucleation. The superior hydrate growth inhibition capability and predictable hydrate melting behavior compared to complex, heterogeneous hydrate melting with Luvicap Bio shows that RmAFP can be a potential natural green kinetic inhibitor for hydrate formation in pipelines.

General information

State: Published
Organisations: Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering
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Pages: 1025-1030
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Main Research Area: Technical/natural sciences

Publication information

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Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
The combined effect of thermodynamic promoters tetrahydrofuran and cyclopentane on the kinetics of flue gas hydrate formation

Carbon dioxide (CO2) capture through hydrate crystallization is a promising method among the new approaches for mitigating carbon emissions into the atmosphere. In this work, we investigate a combination of tetrahydrofuran (THF) and cyclopentane (CP) on the kinetics of flue gas (CO2:20 mol %/N2) hydrate formation using a rocking cell apparatus. Hydrate formation and decomposition kinetics were investigated by constant cooling (hydrate nucleation temperature) and isothermal (hydrate nucleation time) methods. Improved (synergistic) hydrate formation kinetics (hydrate nucleation and growth) were observed when THF and CP were present together compared to the individual THF and CP systems. Moreover, the complete hydrate decomposition temperature of CO2/N2/CP/THF hydrate was found to be slightly higher compared to the individual promoter (CO2/N2/CP and CO2/N2/THF) systems. The combined use of these two promoters is favorable both thermodynamically and kinetically for hydrate formation from flue gas.

General information
State: Published
Organisations: Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering
The contribution of glucagon in an Artificial Pancreas for people with type 1 diabetes

The risk of hypoglycemia is one of the main concerns in treatment of type 1 diabetes (T1D). In this paper we present a head-to-head comparison of a currently used insulin-only controller and a prospective bihormonal controller for blood glucose in people with T1D. The bihormonal strategy uses insulin to treat hyperglycemia as well as glucagon to ensure fast recovery from hypoglycemic episodes. Two separate model predictive controllers (MPC) based on patient-specific models handle insulin and glucagon infusion. In addition, the control algorithm consists of a Kalman filter and a meal time insulin bolus calculator. The feedback is obtained from a continuous glucose monitor (CGM). We implement a bihormonal simulation model with time-varying parameters available for 3 subjects to compare the strategies. We consider a protocol with 3 events - a correct mealtime insulin bolus, a missed bolus and a bolus overestimated by 60%. During normal operation both strategies provide similar results. The contribution of glucagon becomes evident after administration of the overestimated insulin bolus. In a 10h period following an overbolused meal, the bihormonal strategy reduces time spent in hypoglycemia in the most severe case by almost 15% (1.5h), outperforming the insulin-only control. Therefore, glucagon contributes to the safety of an Artificial Pancreas.

General information
State: Published
Organisations: Department of Applied Mathematics and Computer Science, Dynamical Systems, Scientific Computing, Center for Energy Resources Engineering, Slovak University of Technology, Copenhagen University Hospital
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Pages: 5097-5102
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DOIs: 10.1109/ACC.2015.7172134
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The effect of divalent ions on the elasticity and pore collapse of chalk evaluated from compressional wave velocity and low-field Nuclear Magnetic Resonance (NMR)

The effects of divalent ions on the elasticity and the pore collapse of chalk were studied through rock-mechanical testing and low-field Nuclear Magnetic Resonance (NMR) measurements. Chalk samples saturated with deionized water and brines containing sodium, magnesium, calcium and sulfate ions were subjected to petrophysical experiments, rock mechanical testing and low-field NMR spectroscopy. Petrophysical characterization involving ultrasonic elastic wave velocities in unconfined conditions, porosity and permeability measurements, specific surface and carbonate content determination and backscatter electron microscopy of the materials were conducted prior to the experiments. The iso-frame model was used to predict the bulk moduli in dry and saturated conditions from the compressional modulus of water-saturated rocks. The effective stress coefficient, as introduced by Biot, was also determined from density and ultrasonic velocities measured on core plugs. Low-field NMR spectroscopy was used in addition to the mechanical testing to prove any changes observed after the saturation related to the surface-to-volume ratio of the pore space in each of the samples or to surface relaxivity. Backscatter-electron (BSE) images were recorded in order to identify the texture of the core plugs under investigation. The experimental results revealed that both elasticity and pore collapse are influenced by the presence of divalent ions in distinct ways. Compressional wave velocities indicate that saturation with water rich in magnesium and calcium ions softens the contact among the mineral grains. Pore collapse strength is deteriorating after
the saturation of chalk with water rich in divalent ions. The presence of calcium and sulfate ions in the saturating fluid results in pore collapse at lower stresses than in the case when samples are saturated with deionized water or sodium chloride solution. Low field NMR spectrometry revealed precipitation of crystals in the pore space of chalk saturated with Mg-rich brine. The precipitation of Mg-carbonates was not used to explain the deteriorating pore collapse strength and effects on the elasticity after the saturation since none of the other plugs saturated with divalent ions (Ca\(^{2+}\) and SO\(_{4}^{2-}\)) experienced it.

**General information**

State: Published  
Organisations: Department of Civil Engineering, Section for Geotechnics and Geology, Center for Energy Resources Engineering  
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Web of Science (2018): Indexed yes  
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Web of Science (2017): Indexed yes  
BFI (2016): BFI-level 1  
Scopus rating (2016): CiteScore 2.56 SJR 0.764 SNIP 1.631  
Web of Science (2016): Indexed yes  
BFI (2015): BFI-level 1  
Scopus rating (2015): SJR 0.801 SNIP 1.652 CiteScore 2.38  
Web of Science (2015): Indexed yes  
BFI (2014): BFI-level 1  
Scopus rating (2014): SJR 0.692 SNIP 1.751 CiteScore 1.95  
Web of Science (2014): Indexed yes  
BFI (2013): BFI-level 1  
Scopus rating (2013): SJR 0.822 SNIP 1.901 CiteScore 1.73  
ISI indexed (2013): ISI indexed yes  
Web of Science (2013): Indexed yes  
BFI (2012): BFI-level 1  
Scopus rating (2012): SJR 0.774 SNIP 1.666 CiteScore 1.42  
ISI indexed (2012): ISI indexed yes  
BFI (2011): BFI-level 1  
Scopus rating (2011): SJR 0.648 SNIP 1.41 CiteScore 1.29  
ISI indexed (2011): ISI indexed yes  
Web of Science (2011): Indexed yes  
BFI (2010): BFI-level 1  
Scopus rating (2010): SJR 0.746 SNIP 1.724  
Web of Science (2010): Indexed yes  
BFI (2009): BFI-level 1  
Scopus rating (2009): SJR 1.072 SNIP 1.852  
Web of Science (2009): Indexed yes  
BFI (2008): BFI-level 1  
Scopus rating (2008): SJR 0.841 SNIP 1.435  
Scopus rating (2007): SJR 0.732 SNIP 1.386  
Scopus rating (2006): SJR 0.92 SNIP 1.387  
Web of Science (2006): Indexed yes  
Scopus rating (2005): SJR 0.784 SNIP 1.052
The equivalent source method as a sparse signal reconstruction

This study proposes an acoustic holography method for sound field reconstruction based on a point source model, which uses the Compressed Sensing (CS) framework to provide a sparse solution. Sparsity implies that the sound field can be represented by a minimal number of non-zero terms, point sources in the case of this model. Sparse solutions can be achieved by \( l_1 \) norm minimization, providing accurate reconstruction and robustness to noise, because favouring sparsity suppresses noisy components. The study addresses the influence of the ill-conditioning of the propagation matrix, which can be a challenge for inverse problems where the energy in the solution vector is much greater than the energy in the observations (particularly in acoustic near-fields). Finally, the study examines the case of spatially extended sources and problems where the sparsity condition is not certainly guaranteed.

Thermodynamic modeling of CO\(_2\) absorption in aqueous N-Methyldiethanolamine using Extended UNIQUAC model

A Thermodynamic model that can predict the behavior of the gas sweetening process over the applicable conditions is of vital importance in industry. In this work, Extended UNIQUAC model parameters optimized for the CO\(_2\)-MDEA-H\(_2\)O system are presented. Different types of experimental data consisting of pure MDEA vapor pressure, vapor-liquid equilibrium (VLE) (total pressure and CO\(_2\) partial pressure), freezing point depression (SLE), excess enthalpy, heat capacity and heat of absorption were used to adjust model parameters. The model was then used to predict the NMR spectroscopic data. The developed model accurately represents thermodynamic and thermal properties of the studied systems. The model parameters are valid in the temperature range from -15 to 200 °C, MDEA mass\% of 5-75 and CO\(_2\) partial pressure of 0-6161.5 kPa.

General information
State: Published
Organisations: Department of Electrical Engineering, Acoustic Technology, Department of Applied Mathematics and Computer Science, Center for Energy Resources Engineering, Scientific Computing
Authors: Fernandez Grande, E. (Intern), Xenaki, A. (Intern)
Number of pages: 10
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Source-ID: 116714771
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Thermodynamic modeling of CO\(_2\) absorption in aqueous N-Methyldiethanolamine using Extended UNIQUAC model
A Thermodynamic model that can predict the behavior of the gas sweetening process over the applicable conditions is of vital importance in industry. In this work, Extended UNIQUAC model parameters optimized for the CO\(_2\)-MDEA-H\(_2\)O system are presented. Different types of experimental data consisting of pure MDEA vapor pressure, vapor-liquid equilibrium (VLE) (total pressure and CO\(_2\) partial pressure), freezing point depression (SLE), excess enthalpy, heat capacity and heat of absorption were used to adjust model parameters. The model was then used to predict the NMR spectroscopic data. The developed model accurately represents thermodynamic and thermal properties of the studied systems. The model parameters are valid in the temperature range from -15 to 200 °C, MDEA mass\% of 5-75 and CO\(_2\) partial pressure of 0-6161.5 kPa.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering, CERE – Center for Energy Resources Engineering, Department of Chemistry
Authors: Sadegh, N. (Intern), Stenby, E. H. (Intern), Thomsen, K. (Intern)
Number of pages: 12
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Main Research Area: Technical/natural sciences
Thermodynamic modeling of hydrogen sulfide absorption by aqueous N-methyldiethanolamine using the Extended UNIQUAC model

Aqueous MDEA is the most commonly used solvent for H2S removal from natural gas. A reliable thermodynamic model is required for the proper design of natural gas sweetening processes. In this study, a rigorous thermodynamic model is developed to represent properties of the H2S-MDEA-H2O ternary system. The Extended UNIQUAC model is used to represent the system behavior. The model is created based on models for the constituent binary subsystems. The developed model provides accurate representation of VLE and heat of absorption for the studied system and subsystem in the temperature range of 0-180°C, H2S partial pressure of 0.0033-8329.71kPa, MDEA mass% of 0-50 and loading range of 0-2.17.

General Information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Center for Energy Resources Engineering, Department of Chemistry, CERE – Center for Energy Resources Engineering
Authors: Sadegh, N. (Intern), Stenby, E. H. (Intern), Thomsen, K. (Intern)
Number of pages: 9
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BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
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Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 2.33 SJR 0.869 SNIP 1.155
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.874 SNIP 0.998 CiteScore 1.99
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 0.982 SNIP 1.248 CiteScore 2.28
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.007 SNIP 1.274 CiteScore 2.31
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.152 SNIP 1.286 CiteScore 2.31
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.034 SNIP 1.234 CiteScore 2.26
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
The role of chemical engineering in medicinal research including Alzheimer’s

Various disciplines of chemical engineering, especially thermodynamics and kinetics, play an important role in medicinal research and this has been particularly recognized during the last 10–15 years (von Stockar and van der Wielen, J Biotechnol 59:25, 1997; Prausnitz, Fluid Phase Equilib 53:439, 1989; Prausnitz, Pure Appl Chem 79:1435, 2007; Dey and Prausnitz, Ind Eng Chem Res 50:3, 2011; Prausnitz, J Chem Thermodynamics 35:21, 2003; Tsivintzelis et al. AIChE J 55:756, 2009). It is expected that during the twenty-first century chemical engineering and especially thermodynamics can contribute as significantly to the life sciences development as it has been done with the oil and gas and chemical sectors in the twentieth century. Moreover, it has during the recent years recognized that thermodynamics can help in understanding diseases like human cataract, sickle-cell anemia, Creuzfeldt- Jacob (“mad cow” disease), and Alzheimer’s which are connected to “protein aggregation.” Several articles in the Perspectives section of prominent chemical engineering journals have addressed this issue (Hall, AIChE J 54:1956, 2008; Vekilov, AIChE J 54:2508, 2008). This work reviews recent applications of thermodynamics (and other areas of chemical engineering) first in drug development and then in the understanding of the mechanism of Alzheimer’s and similar diseases.

General information
State: Published
Organisations: Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Ressources Engineering
Authors: Kontogeorgis, G. M. (Intern)
Pages: 57-62
Publication date: 2015

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Publisher: Springer
Trends in energy supply integration: Geothermal Energy

General information
State: Published
Organisations: Department of Civil Engineering, Section for Geotechnics and Geology, Center for Energy Resources Engineering, Danish Geothermal District Heating
Authors: Fabricius, I. L. (Intern), Berg Lorenzen, S. (Ekstern), Mahler, A. (Ekstern), Røgen, B. (Ekstern)
Pages: 65-67
Publication date: 2015

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Title of host publication: DTU International Energy Report 2015: Energy systems integration for the transition to non-fossil energy systems
Publisher: Technical University of Denmark (DTU)
Editors: Hvidtfeldt Larsen, H., Sønderberg Petersen, L.
ISBN (Print): 978-87-550-3970-4
Main Research Area: Technical/natural sciences
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We develop an approach to coupling between viscous flows of the two phases in porous media, based on the Maxwell–Stefan formalism. Two versions of the formalism are presented: the general form, and the form based on the interaction of the flowing phases with the interface between them. The last approach is supported by the description of the flow on the mesoscopic level, as coupled boundary problems for the Brinkmann or Stokes equations. It becomes possible, in some simplifying geometric assumptions, to derive exact expressions for the phenomenological coefficients in the Maxwell–Stefan transport equations. Sample computations show, among other, that apparent relative permeabilities are dependent on the viscosity ratio; that the overall mobility of the phases decreases compared to the standard Buckley–Leverett formalism; and that the effect is determined by the parameter determining the “degree of mixing” between the flowing phases. Comparison to the available experimental data on the steady-state two-phase relative permeabilities is presented.

General information
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Organisations: Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering
Authors: Shapiro, A. (Intern)
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Accounting for imperfect forward modeling in geophysical inverse problems — Exemplified for crosshole tomography

Inversion of geophysical data relies on knowledge about how to solve the forward problem, that is, computing data from a given set of model parameters. In many applications of inverse problems, the solution to the forward problem is assumed to be known perfectly, without any error. In reality, solving the forward model (forward-modeling process) will almost always be prone to errors, which we referred to as modeling errors. For a specific forward problem, computation of crosshole tomographic first-arrival traveltimes, we evaluated how the modeling error, given several different approximate forward models, can be more than an order of magnitude larger than the measurement uncertainty. We also found that the
modeling error is strongly linked to the spatial variability of the assumed velocity field, i.e., the a priori velocity model. We discovered some general tools by which the modeling error can be quantified and cast into a consistent formulation as an additive Gaussian observation error. We tested a method for generating a sample of the modeling error due to using a simple and approximate forward model, as opposed to a more complex and correct forward model. Then, a probabilistic model of the modeling error was inferred in the form of a correlated Gaussian probability distribution. The key to the method was the ability to generate many realizations from a statistical description of the source of the modeling error, which in this case is the a priori model. The methodology was tested for two synthetic ground-penetrating radar crosshole tomographic inverse problems. Ignoring the modeling error can lead to severe artifacts, which erroneously appear to be well resolved in the solution of the inverse problem. Accounting for the modeling error leads to a solution of the inverse problem consistent with the actual model. Further, using an approximate forward modeling may lead to a dramatic decrease in the computational demands for solving inverse problems.

General information
State: Published
Organisations: Center for Energy Resources Engineering, National Space Institute, Mathematical and Computational Geoscience, Department of Applied Mathematics and Computer Science, Aarhus University
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Number of pages: 21
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BFI (2016): BFI-level 1
Scopus rating (2016): SJR 1.122 SNIP 1.143 CiteScore 1.53
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.472 SNIP 1.933 CiteScore 2.03
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.413 SNIP 1.434 CiteScore 1.9
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.658 SNIP 2.105 CiteScore 2.25
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.693 SNIP 1.837 CiteScore 2.04
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 2.141 SNIP 1.729 CiteScore 2.51
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.755 SNIP 1.716
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.659 SNIP 2.661
Web of Science (2009): Indexed yes
A Comprehensive Framework for Surfactant Selection and Design for Emulsion Based Chemical Product Design

The manufacture of emulsified products is of increasing interest in the consumer oriented chemical industry. Several cosmetic, household and pharmaceutical products are in the emulsified form when sold and/or they are expected to form an emulsion when used. Therefore, there is a need for the development of a methodology and relevant tools in order to spare time and resources in the design of emulsion-based chemical products, so that the products can reach the market faster and at a reduced cost. The understanding and modeling of the characteristic behavior of emulsions and their peculiar ingredients is consequently necessary to tackle this problem with computer-aided methods and tools. A comprehensive framework for the selection and design of surfactants, the main responsible for the formation and the stability of emulsions, is presented here together with the modeling of the cloud point, a key-property of nonionic surfactants, with a group-contribution model. The mathematical formulation of a standard product design problem is presented, together with the list of both the pure component properties (related to nonionic surfactants) and the mixture properties (relevant to the overall products as an emulsion) needed for the solution of the design algorithm. These models are then applied together with established predictive models for pure component properties of ionic surfactants and for standard mixture properties such as the density, the viscosity, the surface and the interfacial tension, but also the type of emulsion expected (through the hydrophilic–lipophilic balance), and its stability (through the hydrophilic–lipophilic deviation), forming a robust chemical product design tool. The application of this framework is highlighted for the design of some emulsion based chemical products.
A Dantzig-Wolfe decomposition algorithm for linear economic model predictive control of dynamically decoupled subsystems

This paper presents a warm-started Dantzig–Wolfe decomposition algorithm tailored to economic model predictive control of dynamically decoupled subsystems. We formulate the constrained optimal control problem solved at each sampling instant as a linear program with state space constraints, input limits, input rate limits, and soft output limits. The objective function of the linear program is related directly to the cost of operating the subsystems, and the cost of violating the soft output constraints. Simulations for large-scale economic power dispatch problems show that the proposed algorithm is significantly faster than both state-of-the-art linear programming solvers, and a structure exploiting implementation of the alternating direction method of multipliers. It is also demonstrated that the control strategy presented in this paper can be tuned using a weighted ℓ₁-regularization term. In the presence of process and measurement noise, such a regularization term is critical for achieving a well-behaved closed-loop performance.

General information
State: Published
Organisations: Department of Applied Mathematics and Computer Science, Scientific Computing, Dynamical Systems, Center for Energy Resources Engineering, DONG Energy A/S
Authors: Sokoler, L. E. (Intern), Standardi, L. (Intern), Edlund, K. (Ekstern), Poulsen, N. K. (Intern), Madsen, H. (Intern), Jørgensen, J. B. (Intern)
Pages: 1225-1236
Publication date: 2014
Main Research Area: Technical/natural sciences

Publication information
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Addition of malodorants to lighter gas: The phase equilibrium properties of mixtures of lighter gas and selected substances

Relevant thermodynamic and phase behavior of mixtures created by adding malodorants to lighter gas to discourage its abuse have been studied. The influence of physical factors such as temperature, pressure and concentration of the selected substances with lighter gas is studied. This work represents one component in a larger study examining the feasibility of adding malodorants to lighter gas and focuses on the physical chemistry or chemical engineering aspects of the problem. An initial set of 27 compounds was selected based on deterrent effect (odor) in order to find suitable additives to lighter gas components. The aim is to find substances that not only have the correct physiological effect (discourage abuse) but also the correct physical behavior upon addition to lighter gas (solubility, phase behavior). Specifically the way the malodorant partitions between the vapor and liquid phase is modeled. Furthermore, addition of the malodorants should not affect the normal use of the lighter. Thus of the 27 initial components chosen, nine were found that could be suitable additives. In this work we used the thermodynamic models COSMOtherm - an activity coefficient model - and Cubic-Plus-Association (CPA) - an equation of state - to model the fluid phase and solubility behavior of the mixtures formed by the various additives with butane.

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This paper presents a decomposition algorithm for solving the optimal control problem (OCP) that arises in Mean-Variance Economic Model Predictive Control of stochastic linear systems. The algorithm applies the alternating direction method of multipliers to a reformulation of the OCP that decomposes into small independent subproblems. We test the decomposition algorithm using a simple power management case study, in which the OCP is formulated as a convex quadratic program. Simulations show that the decomposition algorithm scales linearly in the number of uncertainty scenarios. Moreover, a parallel implementation of the algorithm is several orders of magnitude faster than state-of-the-art convex quadratic programming algorithms, provided that the number of uncertainty scenarios is large.
A low energy aqueous ammonia CO₂ capture process

The most pressing challenges regarding the use of ammonia for CO2 capture are the precipitation limitation and the energy penalty of solvent regeneration. Precipitation-free operation is a vital task since solids may cause the shutdown of the plant. Precipitation and slurry formation can be avoided by increasing temperature and L/G ratio but this leads to higher heat consumption, jeopardizing the economic feasibility. Here we developed, investigated, and optimized a novel CO₂ capture process design using aqueous ammonia as solvent. The proposed configuration replaces the traditional stripper for solvent based CO₂ capture with a thermal decomposition reactor. The overall energy penalty is reduced at the expense of introducing a solid handling section which consists of a saturation reactor, a crystallizer and a belt filter. The feasibility of the present approach is demonstrated by simulation. Flow-sheet calculations are performed in Aspen Plus using the extended UNIQUAC thermodynamic model for vapor-liquid-solid equilibria and for thermal properties calculation of the CO₂ -NH₃-H₂O system. The simulation results show that the specific regeneration duty of the novel capture alternative is comparable with existing aqueous ammonia CO₂ capture processes. Moreover, the thermal reactor can operate at 1 bar and 86 °C, therefore the NH₃ regeneration temperature is reduced by approximately 50 °C. The integration of low- and mid- temperature waste heat becomes possible which can greatly improve the economics of the process. The present capture alternative is especially convenient for power plants but is also beneficial for the cement, steel and aluminum industry. Special attention is given to the ammonia slip prediction. The calculations substantiate that the slip above the absorber is 0.1 mol % after washing with the rich solution and it reduces below 100 ppm by washing with low temperature water.
A Mean-Variance Criterion for Economic Model Predictive Control of Stochastic Linear Systems

Stochastic linear systems arise in a large number of control applications. This paper presents a mean-variance criterion for economic model predictive control (EMPC) of such systems. The system operating cost and its variance is approximated based on a Monte-Carlo approach. Using convex relaxation, the tractability of the resulting optimal control problem is addressed. We use a power management case study to compare different variations of the mean-variance strategy with EMPC based on the certainty equivalence principle. The certainty equivalence strategy is much more computationally efficient than the mean-variance strategies, but it does not account for the variance of the uncertain parameters. Openloop simulations suggest that a single-stage mean-variance approach yields a significantly lower operating cost than the certainty equivalence strategy. In closed-loop, the single-stage formulation is overly conservative, which results in a high operating cost. For this case, a two-stage extension of the mean-variance approach provides the best trade-off between the expected cost and its variance. It is demonstrated that by using a constraint back-off technique in the specific case study, certainty equivalence EMPC can be modified to perform almost as well as the two-stage mean-variance formulation. Nevertheless, we argue that the mean-variance approach can be used both as a strategy for evaluating less computational demanding methods such as the certainty equivalence method, and as an individual control strategy when heuristics such as constraint back-off do not perform well.
A mean–variance objective for robust production optimization in uncertain geological scenarios

In this paper, we introduce a mean–variance criterion for production optimization of oil reservoirs and suggest the Sharpe ratio as a systematic procedure to optimally trade-off risk and return. We demonstrate by open-loop simulations of a two-phase synthetic oil field that the mean–variance criterion is able to mitigate the significant inherent geological uncertainties better than the alternative certainty equivalence and robust optimization strategies that have been suggested for production optimization. In production optimization, the optimal water injection profiles and the production borehole pressures are computed by solution of an optimal control problem that maximizes a financial measure such as the Net Present Value (NPV). The NPV is a stochastic variable as the reservoir parameters, such as the permeability field, are stochastic. In certainty equivalence optimization, the mean value of the permeability field is used in the maximization of the NPV of the reservoir over its lifetime. This approach neglects the significant uncertainty in the NPV. Robust optimization maximizes the expected NPV over an ensemble of permeability fields to overcome this shortcoming of certainty equivalence optimization. Robust optimization reduces the risk compared to certainty equivalence optimization because it considers an ensemble of permeability fields instead of just the mean permeability field. This is an indirect mechanism for risk mitigation as the risk does not enter the objective function directly. In the mean–variance bi-criterion objective function risk appears directly, it also considers an ensemble of reservoir models, and has robust optimization as a special extreme case. The mean–variance objective is common for portfolio optimization problems in finance. The Markowitz portfolio optimization problem is the original and simplest example of a mean–variance criterion for mitigating risk. Risk is mitigated in oil production by including both the expected NPV (mean of NPV) and the risk (variance of NPV) for the ensemble of possible reservoir models. With the inclusion of the risk in the objective function, the Sharpe ratio can be used to compute the optimal water injection and production borehole pressure trajectories that give the optimal return–risk ratio. By simulation, we investigate and compare the performance of production optimization by mean–variance optimization, robust optimization, certainty equivalence optimization, and the reactive strategy. The optimization strategies are simulated in open-loop without feedback while the reactive strategy is based on feedback. The simulations demonstrate that certainty equivalence optimization and robust optimization are risky strategies. At the same computational effort as robust optimization, mean–variance optimization is able to reduce risk significantly at the cost of slightly smaller return. In this way, mean–variance optimization is a powerful tool for risk management and uncertainty mitigation in production optimization.
A new approach to model strain change of gelled waxy crude oil under constant stress
Deforation of gelled waxy crude oil with loaded stress is worthy of research for the flow assurance of pipelining system. A dispersion parameter was introduced to characterize the disruption degree of wax crystal structure in crude oil with shear action. Based on fractional calculus theory, a rheological model incorporating dispersion parameter was proposed to describe creep of gelled waxy crude. A discrete and numerical algorithm was proposed to solve the model. Combining with the experimental results of five kinds of waxy crude oil, the model parameters were regressed and found to change monotonously with test temperature. Multiple creep curves of gelled waxy crude oil at a certain temperature can be described with this model.
A new aqueous activity model for geothermal brines in the system Na-K-Ca-Mg-H-Cl-SO4-H2O from 25 to 300 degrees C

A revised formulation (named REUNIQUAC) of the Extended Universal QUasiChemical (EUNIQUAC) activity model has been developed, which fits excess thermodynamic properties of binary and selected aqueous ternary electrolyte solutions in the system Na-K-Ca-Mg-H-Cl-SO4-H2O over temperatures from 298 to 573 K and concentrations to 5 molal (or up to saturation if solubility is below 5 molal) for saturated water vapor conditions. Compared to the original EUNIQUAC model, REUNIQUAC employs an extended version of the Debye-Huckel model using effective ionic radii of solute species, a concentration dependence of a UNIQUAC parameter, an additional empirical term for strongly complexing salts, as well as a simple quadratic temperature dependence of the fitting parameters. REUNIQUAC considers only pairwise interactions between solute species, as opposed to the Pitzer activity model, which additionally needs to account for ternary interactions. Since REUNIQUAC uses also species-specific parameters, extension of the existing parameter set to solutions that are composed of different combinations of the fitted species, is straightforward, and involves only the parameterization of the pairwise interaction terms. All systems could be fitted with accuracy comparable to the Pitzer model or better, although with much fewer parameters.

General information
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An Integrated Methodology for Emulsified Formulated Product Design

The consumer oriented chemical based products are used every day by millions of people. They are structured products constituted of numerous chemicals, and many of them, especially household and personal care products, are emulsions where active ingredients, solvents, additives and surfactants are mixed together to determine the desired emulsified product. They are still mainly designed and analysed through trial - and - error based exper- imental techniques, therefore a systematic approach , integrating model-based as well a s experiment - based techniques, for design of these products could significantly reduce both time and cost connected to product development by doing only the necessary experi- ments , and ensuring chances for innovation . The main contribution of this project i s the development of an integrated methodology for the design of emulsified formulated products. The methodology consists of three stages: the problem definition stage, the model - based design stage, and the experiment - based verification stage. In the probl em definition stage, the consumer needs are trans- lated into a set of target thermo - physical properties and into a list of categories of ingre- dients that are to be included in the formulation. In the model - based design stage, struc- tured databases, dedicated algorithms and a property model library are employed for de- signing a candidate base case formulation. Finally, in the experiment - based verification stage, the properties and performances of the proposed formulation are measured by means of tailor - made exp eriments. The formulation is then validated or, if necessary, re- fined thanks to a systematic list of action. The problem definition stage relies on a robust knowledge base, which needs to system- atically generate quantitative, useful input information for t he model - based stage, starting from the consumer assessments. In the model - based stage, comprehensive chemical da- tabases, consistent property models and a dedicated algorithm for the design of emulsified solvent mixtures are needed. Finally, for the experi ment - based stage, an efficient planning of the experiments is required, together with the systematic generation of a list of actions to be taken, in case some of the experiments do not validate the candidate formulation generated in the previous stage. All the above mentioned issues are addressed in this PhD work: the necessary property models have been retrieved and organized in a model library; new property models have been developed for a set of thermo - physical properties of surfactants; a robust, system atic knowledge - base has been developed in relation to emulsified formulated products; chem- ical databases have been improved and generated; and an algorithm for the model - based design of emulsified solvent mixtures has been developed. All these tools have b een im- plemented as a new template in the virtual Product - Process Design laboratory software. To illustrate the application of the proposed methodology, three case studies have been developed. For one of these case studies, the whole methodology has been ap plied, while for the other two, only the first two stages and part of the experiment - based verification iv stage have been applied, that is, the experimental work has been planned, a list of actions has been generated, but no actual measurement has been taken .
Antifreeze activity enhancement by site directed mutagenesis on an antifreeze protein from the beetle Rhagium mordax.

The ice binding motifs of insect antifreeze proteins (AFPs) mainly consist of repetitive TxT motifs aligned on a flat face of the protein. However, these motifs often contain non-threonines that disrupt the TxT pattern. We substituted two such disruptive amino acids located in the ice binding face of an AFP from Rhagium mordax with threonine. Furthermore, a mutant with an extra ice facing TxT motif was constructed. These mutants showed enhanced antifreeze activity compared to the wild type at low concentrations. However, extrapolating the data indicates that the wild type will become the most active at concentrations above 270μmol.
Application of Constrained Linear MPC to a Spray Dryer

In this paper we develop a linear model predictive control (MPC) algorithm for control of a two stage spray dryer. The states are estimated by a stationary Kalman filter. A non-linear first-principle engineering model is developed to simulate the spray drying process. The model is validated against experimental data and able to precisely predict the temperatures, the air humidity and the residual moisture in the dryer. The MPC controls these variables to the target and reject disturbances. Spray drying is a cost-effective method to evaporate water from liquid foods and produces a free flowing powder. The main challenge of spray drying is to meet the residual moisture specification and prevent powder from sticking to the chamber walls. By simulation we compare the performance of the MPC against the conventional PID control strategy. During an industrially recorded disturbance scenario, the MPC increases the production rate by 7.9%, profit of production by 8.2% and the energy efficiency by 4.1% on average.
A Realistic Process Example for MIMO MPC based on Autoregressive Models

Advanced controllers such as model predictive control are in use for a wide range of applications in the process industry. The potential utilization of such advanced predictive controllers is far from exhausted. One barrier for more widespread implementation is the lack of simple methodologies for advanced control design development which may be used by non-experts in control theory. This paper presents and illustrates the use of a simple methodology to design an offset-free MPC based on ARX models. Hence a mechanistic process model is not required. The forced circulation evaporator by Newell and Lee is used to illustrate the offset-free MPC based on ARX models for a nonlinear multivariate process.

General information
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A Reduced Dantzig-Wolfe Decomposition for a Suboptimal Linear MPC

Linear Model Predictive Control (MPC) is an efficient control technique that repeatedly solves online constrained linear programs. In this work we propose an economic linear MPC strategy for operation of energy systems consisting of multiple and independent power units. These systems cooperate to meet the supply of power demand by minimizing production costs. The control problem can be formulated as a linear program with block-angular structure. To speed-up the solution of the optimization control problem, we propose a reduced Dantzig-Wolfe decomposition. This decomposition algorithm computes a suboptimal solution to the economic linear MPC control problem and guarantees feasibility and stability. Finally, six scenarios are performed to show the decrease in computation time in comparison with the classic Dantzig-Wolfe algorithm.

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Organisations: Department of Applied Mathematics and Computer Science, Scientific Computing, Dynamical Systems, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering, Centre for IT-Intelligent Energy Systems in Cities
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Assessment of Dynamic Flow, Pressure and Geomechanical Behaviour of a CO₂ Storage Complex

The increasing global temperature is of much concern to the present and future society and is drawing much attention to climate change causes and consequently, significant efforts are being made to mitigate global emissions of greenhouse gases from the atmosphere as one of the main causes. Carbon dioxide (CO₂) is the primary greenhouse gas emitted through human activities. Over 7,500 large CO₂ emission sources (above 0.1 million tons CO₂ year⁻¹) have been identified (IPCC, 2005). These sources are distributed geographically around the world but four clusters of emissions can be observed: in North America (the Midwest and the eastern freeboard of the USA), North West Europe, South East Asia (eastern coast) and Southern Asia (the Indian sub-continent). One of the ways in which global emission of CO₂ can be reduce is by capturing large volumes of CO₂ from point sources (carbon emitters such as coal-fired power plants) and injecting it into deep formations (e.g., saline aquifers, oil and gas reservoirs, and coalbeds) for storage. This process has drawn increasing consideration as a promising mitigation method that is economically possible. Deep saline aquifers offer the largest storage potential of all the geological CO₂ storage options and are widely distributed throughout the globe in all sedimentary basins. CO₂ storage cannot have a significant impact on reducing atmospheric levels of greenhouse gases if the amounts of CO₂ injected and sequestered underground is not extremely large. However, there is concern that storing extremely large amounts of supercritical CO₂ in deep formations will introduce additional fluids that may cause pressure changes and displacement of native brines thereby affecting subsurface volumes that can be significantly larger than the CO₂ plume itself. If this happens it will be of great environmental concern especially to the ground water and other subsurface resources implying that quantifying pressure changes in CO₂ sites is very important for monitoring purposes in order to prevent this phenomenon.

Large scale CO₂ storage has previously been considered for the Vedsted structure located in the Northern part of Jylland in Denmark. In the Vedsted site the primary caprock is the 530 m thick Fjerritslev Formation sealing the Gassum Formation. The Fjerritslev Formation extends from the Norwegian-Danish Basin to the Northeast and North Sea Central Graben to the Southwest. The magnitude of pressure buildup and transmission from the reservoir into the surrounding formations will depend on the properties (compressibility and permeability) and thickness of the sealing rock and presence of faults. Pressure buildup in the Gassum reservoir and transmission to the shallower Chalk Group where the brine-fresh water interface resides need to be investigated and quantified through simulation studies as part of site qualification, as overpressure can push brine into the fresh water zone and thereby affecting aquifer performance.

In order to estimate the sealing potential and rock properties, samples from the deep wells, Vedsted-1, in Jylland and Stenillle-2 and -5 on Sjælland were studied and compared to samples from Skjold Flank-1n the Central North Sea. Mineralogical analysis based on X-ray diffractometry (XRD) of shale cuttings samples obtained from the three different locations show a clear trend in composition from the Northeast presently onshore of the Norwegian-Danish Basin where we encounter a more silty shale with up to 50% quartz content to less silty shale of about 30% quartz content in the Southwest, offshore section of the Central Graben. Iillite and kaolinite dominate the clay fraction. The equivalent pore radius that links permeability and porosity of a porous medium was calculated from specific surface and porosity data measured in the laboratory. In this study we demonstrate that elastic moduli as calculated from bulk density and velocity of elastic waves relate to equivalent pore radius from logging data. We found exponential relationships between equivalent pore radius and elastic moduli, and these empirical relationships were used to calculate equivalent pore radius for the Cenozoic, Cretaceous and Jurassic shale sections in Skjold Flank-1 well from elastic moduli, calculated from sonic velocity and density logs. The calculated equivalent pore radius logs vary from 27 nm at 500 m to 13 nm at 2000 m within Cenozoic shale and from 12 nm to about 6 nm in the deeper Cretaceous and Jurassic shale intervals. Porosity of shale was measured from three independent methods including helium porosimetry (HPMI), mercury injection capillary pressure (MICP) and nuclear magnetic resonance (NMR) and the results on same material show that MICP porosity is 6% to 10% points lower than HPMI or NMR porosity. Compressibility from uniaxial loading and velocity of elastic waves were measured simultaneously on saturated samples under drained condition at room temperature. Uniaxial loading causes both elastic and plastic deformation at low stress, but unloading at stress corresponding to in situ stress gives stiffer material with high elastic moduli close to values calculated from mass density and velocity of elastic waves. This result indicates that shale is significantly stiffer in situ than normally assumed in geotechnical modelling. Permeability can be predicted from elastic moduli and from combined MICP and NMR data. The predicted permeability from BET specific surface using Kozeny’s formulation for these shales being rich in silt and kaolinite fall in the same order of magnitude as measured permeability from constant rate of strain (CRS) experiments, but is two to
Assessment of Model Predictive and Adaptive Glucose Control Strategies for People with Type 1 Diabetes

This paper addresses overnight blood glucose stabilization in people with type 1 diabetes using a Model Predictive Controller (MPC). We use a control strategy based on an adaptive ARMAX model in which we use a Recursive Extended Least Squares (RELS) method to estimate parameters of the stochastic part. We compare this model structure with an autoregressive integrated moving average with exogenous input (ARIMAX) structure, and with an autoregressive moving average with exogenous input (ARMAX) model, i.e. without an integrator. Additionally, safety layers improve the controller robustness and reduce the risk of hypoglycemia. We test our control strategies on a virtual clinic of 100 randomly generated patients with a representative inter-subject variability. This virtual clinic is based on the Hovorka model. We consider the case where only half of the meal bolus is administered at mealtime, and the case where the insulin sensitivity varies during the night. The simulation results demonstrate that the adaptive control strategy can reduce the risks of hypoglycemia and hyperglycemia during the night.

General information

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A Tuning Approach for Offset-free MPC with Conditional Reference Adaptation.

Model predictive control has become a widely accepted strategy in industrial applications in recent years. Often mentioned reasons for the success are the optimization based on a system model, consideration of constraints and an intuitive tuning process. However, as soon as unknown disturbances or model plant mismatch have to be taken into account the tuning effort to achieve offset-free tracking increases. In this work a novel approach for offset-free MPC is presented, which divides the tuning in two steps, the setup of a nominal MPC loop and an external reference adaptation. The inner nominal loop addresses the performance targets in the nominal case, decouples the system and essentially leads to a first order response. The second outer loop enables offset-free tracking in case of unknown disturbances and consists of feedback controllers adapting the reference. Due to the mentioned properties these controllers can be tuned separately and by known guidelines. To address conditions with active input constraints, additionally a conditional reference adaptation scheme is introduced. The tuning strategy is evaluated on a simulated linear Wood-Berry binary distillation column example.

Benchmarking and comparing first and second generation post combustion CO2 capture technologies

The Octavius FP7 project focuses on demonstration of CO2 capture for zero emission power generation. As part of this work many partners are involved using different rate based simulation tools to develop tomorrow's new power plants. A benchmarking is performed, in order to synchronize accuracy and quality control the used modeling tools.

General information

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In this paper we present a bihormonal control system that controls blood glucose in people with type 1 diabetes (T1D). We use insulin together with glucagon to mitigate the negative effects of hyper- and hypoglycemia. The system consists of a Kalman filter, a micro-bolus insulin and glucagon infusion MPC, a mealtime bolus calculator and a CGM providing feedback to the controller. The controller employs a patient data-based prediction model with ARMAX structure. We test the controller using a bihormonal model with time-varying parameters for 3 subjects and compare its performance to a system with an identical insulin MPC, but a glucagon PD controller. The key contribution of the bihormonal MPC is the efficiency of glucagon use. We consider scenarios where the meals are estimated correctly or overestimated and where the insulin sensitivity increases. Both solutions provide tight glucose control. According to the simulations, the bihormonal MPC requires on average 30% less glucagon than the system with a PD controller.
Burial stress and elastic strain of carbonate rocks

Burial stress on a sediment or sedimentary rock is relevant for predicting compaction or failure caused by changes in, e.g., pore pressure in the subsurface. For this purpose, the stress is conventionally expressed in terms of its effect: “the effective stress” defined as the consequent elastic strain multiplied by the rock frame modulus. We cannot measure the strain directly in the subsurface, but from the data on bulk density and P-wave velocity, we can estimate the rock frame modulus and Biot’s coefficient and then calculate the “effective vertical stress” as the total vertical stress minus the product of pore pressure and Biot’s coefficient. We can now calculate the elastic strain by dividing “effective stress” with the rock frame modulus. This facilitates the discussion of the deformation mechanisms. The principle is illustrated by comparing carbonate sediments and sedimentary rocks from the North Sea Basin and three oceanic settings: a relatively shallow water setting dominated by coarse carbonate packstones and grainstones and two deep water settings dominated by fine-grained carbonate mudstones and wackestones.

General information

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Caprock compressibility and permeability and the consequences for pressure development in CO₂ storage sites

Large scale CO₂ storage has previously been considered for the Vedsted structure located in the Northern part of Jylland in Denmark. Pressure buildup in the Gassum reservoir and transmission to the shallower Chalk Group where the brine-fresh water interface resides need to be investigated as part of site qualification, as overpressure can push brine into the fresh water zone and thereby affecting aquifer performance. Pressure transmission from the reservoir into the surrounding formations, when fractures and faults are ignored, will depend on the properties and thickness of the sealing rock. The most important property to be considered is caprock compressibility and permeability. Laboratory experiments on centimeter-scale plugs and dynamic sonic velocity data from relevant shale formations in Denmark indicate that shale compressibility is lower than often assumed for reservoir simulation studies. The measured compressibility for the Fjerritslev Formation is 0.5×10⁻⁵ bar⁻¹, which is an order of magnitude lower than the standard compressibility (4.5×10⁻⁵ bar⁻¹) normally used for reservoir simulation studies. The consequences of this lower compressibility are investigated in a simulation case study and the results indicate that higher overpressure is created in the reservoir and the caprock. Overestimating caprock compressibility can therefore underestimate overpressure within the storage and sealing formations and this can have significant implication in the presence of highly permeable fractures and faults. The caprock permeability is measured on core samples using a geotechnical method of constant rate of strain (CRS) experiments which seem to match the modeled permeability data for the Fjerritslev Formation. We found an average vertical permeability of 0.1μD for the Fjerritslev Formation from the samples measured. The sensitivity of pressure development for the caprock permeability has been studied by varying from one to three orders of magnitude higher and one to two orders of magnitude lower than the measured permeability of 0.1μD. Injecting 60 million tons (Mt) of CO₂ at a rate of 1.5Mt/year into the Gassum Formation for 40 years indicates that, with permeability above 1.0μD, overpressure can be transmitted through the 530m thick Fjerritslev Formation caprock and further up into the overburden layers. © 2014 Elsevier Ltd.
Changes in Specific Surface as observed by NMR, caused by saturation of Chalk with porewater bearing divalent ions

Nuclear Magnetic Resonance (NMR) spectrometry has proved to be a good technique for determining the petrophysical properties of reservoir rocks; such as porosity and pore size distribution. We investigated how pore water rich in divalent ions affect the NMR signal from chalk with two different depositional textures. We compared two cases. The first experiments on outcrop chalk with high salinity brines showed that saturation with divalent ions (Mg$^{2+}$, Ca$^{2+}$ and SO$_4^{2-}$) cause major shifts in the $T_2$ distribution curve, probably due to precipitation in the pore space. In a second set of experiments, fluid samples where precipitation takes place were found to show shifts in the $T_2$ relaxation curve due to the creation of crystals. We were able to identify how differences in the rock texture and precipitants within the pore space may affect the transverse relaxation time by altering the surface-to-volume ratio of the pore space. The results of this work could benefit the ongoing study on the optimization of the water composition for Enhanced Oil Recovery (EOR) methods and shed light on how it can affect the mechanical and physical properties of the rock.
Compressibilities and viscosities of reference, vegetable, and synthetic gear lubricants

Nowadays, one of the primary choices of base oils for environmentally aware lubricants is vegetable oils. This is due to their good natural biodegradability and very low toxicity in combination with very good lubricity characteristics. The development of new vegetable-based lubricants requires the knowledge of their thermophysical properties such as their viscosity or density, among others. Regarding this issue, in this work, we have carried out density measurements between 278.15 and 398.15 K and pressures up to 120 MPa and calculated the isothermal compressibility and isobaric thermal expansivity values of six gear lubricants, two of them reference mineral oils and the other four developed biodegradable oils based in high oleic sunflower oil or in synthetic esters. It was found that all of the lubricants have both similar compressibilities and similar expansivities. Dowson and Higginson, Zhu and Wen, Jacobson and Vinet equations of state predict the experimental density values with absolute average deviations (AADs), that is, AAD % lower than 0.3, 0.4, and 0.6%, respectively, whereas Tammann-Tait and the modified Tait equations correlate these experimental densities with AAD % of 0.02 and 0.06%. Dowson and Higginson and Zhu and Wen equations of state do not predict well the isothermal compressibilities, with AAD % being around 45% for both equations. Moreover, the viscosities were measured in the temperature range from 278.15 to 373.15 K at atmospheric pressure for these oils, and the viscosity index was also determined. New formulated oils present the highest viscosity indexes and the lowest viscosity data at low temperatures; therefore, they become the most suitable for machinery cold start. © 2014 American Chemical Society.
COMPRESSIBILITY, Atmospheric pressure, Biodegradation, Compressibility, Equations of state, Isotherms, Lubricants, Machinery, Thermodynamic properties, Absolute average deviation, Bio-degradable oil, High-oleic sunflower oil, Isobaric thermal expansivities, Isothermal compressibility, Low temperatures, Synthetic esters, Temperature range, Viscosity

DOIs:
Conditional Reference Adaptation for Offset-free MPC

Model predictive control has become a widely accepted strategy in industrial applications in the recent years. Often mentioned reasons for the success are the optimization based on a system model, consideration of constraints and an intuitive tuning process. However, as soon as unknown disturbances or model plant mismatch have to be taken into account the tuning effort to achieve offset-free tracking increases. In this work a novel approach for offset-free MPC is presented, which divides the tuning in two steps, the setup of a nominal MPC loop and an external reference adaptation. The inner nominal loop addresses the performance targets in the nominal case, decouples the system and essentially leads to a first order response. The second outer loop enables offset-free tracking in case of unknown disturbances and consists of feedback controllers adapting the reference. Due to the mentioned properties these controllers can be tuned separate and by known guidelines. To address conditions with active input constraints, additionally a conditional reference adaptation scheme is introduced. The tuning strategy is evaluated on a simulated linear Wood-Berry binary distillation column example.

General information
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Organisations: Center for Energy Resources Engineering, Department of Applied Mathematics and Computer Science, Scientific Computing, Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Johannes Kepler University of Linz
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Crossflow and water banks in viscous dominant regimes of waterflooding
Understanding the crossflow in multilayered reservoirs is of great importance for designing mobility control methods for enhanced oil recovery. The authors reveal saturation profiles in stratified reservoirs to study the interlayer communication in the viscous dominant regime. The displacement profiles are more even and smoother in a communicating layer-cake reservoir than in a noncommunicating one. Water banks and transition zones may be observed. Analysis indicates that the phenomena are attributed to the enhanced crossflow due to large mobility ratios (water-oil). The mobility control techniques that take advantage of crossflow between layers may be more efficient with large mobility ratios. © 2014 Copyright Taylor & Francis Group, LLC.

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Organisations: Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering, Department of Chemistry, Haldor Topsoe AS
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Crystallization Kinetics within a Generic Modeling Framework

A new and extended version of a generic modeling framework for analysis and design of crystallization operations is presented. The new features of this framework are described, with focus on development, implementation, identification, and analysis of crystallization kinetic models. Issues related to the modeling of various kinetic phenomena like nucleation, growth, agglomeration, and breakage are discussed in terms of model forms, model parameters, their availability and/or estimation, and their selection and application for specific crystallization operational scenarios under study. The advantages of employing a well-structured model library for storage, use/reuse, and analysis of the kinetic models are highlighted. Examples illustrating the application of the modeling framework for kinetic model discrimination related to simulation of specific crystallization scenarios and for kinetic model parameter estimation are presented.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering, CERE – Center for Energy Resources Engineering, CAPEC-PROCESS
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Scopus rating (2013): SJR 0.724 SNIP 1.048 CiteScore 1.83
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BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.624 SNIP 0.723
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.582 SNIP 0.722
BFI (2008): BFI-level 1
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Web of Science (2008): Indexed yes
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Scopus rating (2006): SJR 0.554 SNIP 0.632
Determination of Matrix Pore Size Distribution in Fractured Clayey Till and Assessment of Matrix Migration of Dechlorinating Bacteria

The pore structure and pore size distribution (PSD) in the clayey till matrix from three Danish field sites were investigated by image analysis to assess the matrix migration of dechlorinating bacteria in clayey till. Clayey till samples had a wide range of pore sizes, with diameters of 0.1–100 μm, and two typical peaks of pore sizes were observed in all clayey till samples. A large area fraction of the individual pores centered around 2 μm in diameter, and another fraction centered around 20 μm. In general, the typical macropore sizes (1 μm < D < 30 μm) in clayeys determined by image analysis account for approximately 30–60% of the total porosity (20–28%), which is within the range of those reported for clayey soils and other clayey deposits in the literature. The pore size, PSD, and interconnectivity of pores in clayey till matrix may play an important role in evaluation of the migration of dechlorinating bacteria between fractures and clayey till matrix. Dechlorinating bacteria are small (0.3–1 μm) and may have the ability to morphologically adapt to space constraints. The results in this paper in combination with recent field data indicate that the migration of dechlorinating bacteria in fractures and into the clayey till matrix is likely, which is of significance for natural and stimulated degradation of chlorinated solvents by reductive dechlorination in clayey tills.

General Information
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Organisations: Department of Environmental Engineering, Water Resources Engineering, Department of Civil Engineering, Section for Geotechnics and Geology, Center for Energy Resources Engineering
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BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.315 SNIP 0.374 CiteScore 0.81
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Scopus rating (2013): SJR 0.368 SNIP 0.541 CiteScore 0.93
In this work, we present a further development and analysis of the Original UNIFAC-CI models for the prediction of vapor-liquid equilibrium (VLE) and solid-liquid equilibrium (SLE) for a wide range of mixtures. Three sets of atom interaction parameters (AIPs) have been regressed. For the first two sets, only VLE experimental data were used in parameter estimation. In the first set, no weighting factors were used for each of the VLE data in the objective function when regressing the AIPs. However, for the second set, the AIPs have been regressed using the so-called QVLE quality factors obtained for each of the VLE data from a quality assessment algorithm (consistency tests) as weighting factors in the objective functions. For the third set of parameters, SLE and VLE data were used in the regression of AIPs. The result of the correlations in terms of deviations errors and predictions using these three sets of regressed parameters are presented, compared and discussed. The significance of adding the QVLE values and SLE systems in the regression of the AIPs are also highlighted. UNIFAC is a model that can be in principle used for both VLE and SLE (as well as other types of phase behavior) calculations. The range of applicability of the predictive UNIFAC-CI is investigated and it is shown to what extent the Original UNIFAC-CI model can successfully predict SLE especially when the needed parameters are missing.
Development of a LSSVM-GC model for estimating the electrical conductivity of ionic liquids

In this communication, an extensive set of 1077 experimental electrical conductivity data for 54 ionic liquids (ILs) was collected from 21 different literature sources. Using this dataset, a reliable least square support vector machine-group contribution (LSSVM-GC) model has been developed, which employs a total of 22 sub-structures in addition to the temperature to represent/predict the electrical conductivity of ILs. In order to distinguish the effects of the anion and cation on the electrical conductivity of ILs, 11 sub-structures related to the chemical structure of anions, and 11 sub-structures related to the chemical structure of cations were implemented. The proposed model produces a low average absolute relative deviation (AARD) of less than 3.3% taking into consideration all 1077 experimental data values.

General information
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Scopus rating (2016): CiteScore 2.79 SJR 0.813 SNIP 1.303
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Web of Science (2015): Indexed yes
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Web of Science (2014): Indexed yes
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BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.933 SNIP 1.614 CiteScore 2.31
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Scopus rating (2011): SJR 0.912 SNIP 1.335 CiteScore 2.12
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.87 SNIP 1.317
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.742 SNIP 1.029
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
This thesis extends the Cubic Plus Association (CPA) equation of state (EoS) to handle mixtures containing ions from fully dissociated salts. The CPA EoS has during the past 18 years been applied to thermodynamic modeling of a wide range of industrially important chemicals, mainly in relation to the oil- and gas sector. One of the strengths of the CPA EoS is that it reduces to the Soave Redlich Kwong (SRK) cubic EoS in the absence of associating compounds and is therefore compatible with existing tools for oil characterization. In a similar fashion, the electrolyte CPA (e-CPA) EoS reduces to the CPA EoS in the absence of electrolytes, making it possible to extend the applicability of the CPA EoS while retaining backwards compatibility and reusing the parameters for non-electrolyte systems. There are many challenges related to thermodynamic modeling of mixtures containing electrolytes, and many different approaches to the development of an electrolyte EoS have been suggested by scientists in the field. However, most of these approaches are focusing on aqueous solutions and cannot easily be extended to handle mixed solvents. Furthermore, the approaches suggested in current literature have rarely been applied to all types of thermodynamic equilibrium calculations relevant to electrolyte solutions. This project has aimed to determine the best recipe to deliver a complete thermodynamic model capable of handling electrolytes in mixed solvents and at a wide range of temperature and pressure. Different terms describing the electrostatic interactions have been compared and it was concluded that the differences between the Debye-Hückel and the "mean spherical approximation" models are negligible. A term accounting for the Gibbs energy of hydration (such as the Born term) must be included in order to provide sufficient driving forces for electrolytes towards the most polar phase. The static permittivity of the mixture was found to be the most important property; yet it was shown that the empirical models suggested by literature could lead to unphysical behavior of the equation of state. A new theoretical model was developed to extend the framework for modeling of the static permittivity to hydrogen-bonding compounds and salts. The model relates the geometrical configuration of hydrogen-bonding dipolar molecules to the Kirkwood g-factor using the Wertheim association model that is included with modern EoS such as CPA or SAFT (Statistical Associating Fluid Theory). This new model was shown to give excellent predictions of the static permittivity of mixtures over wide ranges of temperature, pressure, and composition and thereby generalizes the handling of electrolytes in mixed solvents in an electrolyte EoS. The CPA EoS was extended with a Debye-Hückel and a Born term to account for the electrostatics along with the new model for the static permittivity. This new e-CPA EoS was parameterized against osmotic coefficient, density, and mean ionic activity coefficient data of pure salts and validated against salt mixture data. The model was then applied to predict: • the solubility of light gases, hydrocarbons, and aromatics in aqueous mixtures and mixed solvents • solid-liquid equilibrium in aqueous salt mixtures and mixed solvents • gas hydrate formation pressures of methane with salts in water+methanol • liquid-liquid and liquid-liquid-liquid equilibrium with water-propan-1-ol-NaCl-octane solutions It was demonstrated that the model has a good potential for applications in relation to e.g. flow assurance during the production of natural gas. The parameterization of electrolyte EoS is of high importance and more work is needed in order to obtain good ion-specific parameters that include interaction parameters with gases and relevant chemicals.
Distribution of gas hydrate inhibitor monoethylene glycol in condensate and water systems: Experimental measurement and thermodynamic modeling using the cubic-plus-association equation of state

The deepwater energy sector represents one of the major growth areas of the oil and gas industry today. To meet the challenges of hydrate formation, corrosion, scaling, and foaming, the oil and gas industry uses many chemicals and their use has increased significantly over the years. To inhibit gas hydrate formation in subsea pipelines, monoethylene glycol (MEG) and methanol are injected in large amounts. It is important to know the distribution of these chemicals in oil and water systems for economical operation of a production facility and environmental perspective. In this work, we present new data for liquid-liquid equilibrium of North Sea condensate + MEG and North Sea condensate + MEG + water systems for temperatures from 303.15 to 323.15 K and atmospheric pressure. These data are successfully modeled using the cubic-plus-association equation of state. © 2014 American Chemical Society.
Economic Optimization of Spray Dryer Operation using Nonlinear Model Predictive Control

In this paper, we investigate an economically optimizing Nonlinear Model Predictive Control (E-NMPC) for a spray drying process. By simulation, we evaluate the economic potential of this E-NMPC compared to a conventional PID based control strategy. Spray drying is the preferred process to reduce the water content for many liquid foodstuffs and produces a free flowing powder. The main challenge in controlling the spray drying process is to meet the residual moisture specifications and avoid that the powder sticks to the chamber walls of the spray dryer. We present a model for a spray dryer that has been validated on experimental data from a pilot plant. We use this model for simulation as well as for prediction in the E-NMPC. The E-NMPC is designed with hard input constraints and soft output constraints. The open-loop optimal control problem in the E-NMPC is solved using the single-shooting method combined with a quasi-Newton Sequential Quadratic Programming (SQP) algorithm and the adjoint method for computation of gradients. The E-NMPC improves the cost of spray drying by 26.7% compared to conventional PI control in our simulations.
Effect of salinity and specific ions on amount of bound water on quartz, calcite and kaolinite, as observed by NMR transverse relaxation time ($T_2$)

General information
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Organisations: Department of Civil Engineering, Section for Geotechnics and Geology, Center for Energy Resources Engineering, Section for Structural Engineering
Authors: Alam, M. M. (Intern), Katika, K. (Intern), Fabricius, I. L. (Intern)
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Effect of temperature on sandstone permeability: Mineral-fluid interaction

Hot water injection in geothermal sandstone aquifers is considered for seasonal energy storage in Denmark. However, an increase in the aquifer temperature might reduce permeability, and thereby increase production costs. An understanding of the factors that control permeability is required in order to address the effects of temperature on permeability. Therefore, different aspects of sandstone permeability are investigated in this research project. Data from a range of sources including: published literature; a database containing over 120 tight gas sandstone samples; new flow-through experiments on Berea sandstone, which is often used as a reference material to reservoir sandstones; and flow-through experiments on Danish Gassum Formation sandstone and Bunter Formation sandstone, were analysed. Polished thin sections were studied by using the electron microscope in order to relate permeability to sandstone texture.

The simple physically based Kozeny (1927) equation, relates permeability to porosity and specific surface per pore volume, or equivalent pore size, for a homogeneous porous medium with a uniform pore size. As pore sizes in sandstones can range from nanometres to micrometres, additional assumptions would be required in order to estimate sandstone permeability based on the Kozeny equation. An effective specific surface area per pore volume for permeability was estimated by using image analysis and pore size distributions from NMR transverse relaxation data. The smaller pores in the pore size distribution appear to control permeability in sandstones with a low clay-free intergranular porosity. Presumably in those sandstones larger intergranular pores are only connected through smaller pores, which therefore limit the flow rate in larger pores. In sandstones where larger intergranular pores do form a connected flow path, the higher permeability in these pores would have the dominant effect on the measured permeability, wherefore the effective specific surface reflects the specific surface of the framework grains.

A characteristic equivalent pore size can also be determined based on the Klinkenberg (1941) procedure, which accounts for effects of permeability of gas slip on the fluid-solid interface by means of several permeability measurements with different pore pressures. A comparison between the equivalent pore sizes as estimated using the Kozeny equation and
the Klinkenberg procedure showed the expected correlation between the two measures, however, differences could be around one order of magnitude. In tight gas sandstones, permeability is often sensitive to net stress, which might change due to the pore pressure change in the Klinkenberg procedure. Besides affecting the Klinkenberg procedure, the combined effect of slip and changes in permeability would affect production during pressure depletion in tight gas sandstone reservoirs; therefore effects of gas slip and net stress on permeability were combined in a model based on the Klinkenberg equation.

A lower permeability to brine than to gas is often observed, which might be due to interaction between the mineral surface and the pore fluid. By modelling a layer of immobile fluid on the fluid-mineral interface permeability to brine was estimated, based on both the pore size distribution from NMR combined with the Kozeny equation and the Klinkenberg procedure. Both methods overestimated the measured brine permeability; this suggests that additional factors, possibly related to clay morphology, contributed to a lower brine permeability.

Thermal expansion would have a negligible effect on permeability as estimated based on the Kozeny equation. Accordingly, a literature survey indicated no effect of heating on permeability in experiments with an inert pore fluid; in tests with distilled water or brine, heating reduced permeability in sandstones containing kaolinite clay minerals. Both heating and reduction of the salinity of the pore fluid can increase the electrical double layer repulsion between quartz grains and kaolinite particles in Berea sandstone, which could lead to kaolinite mobilisation and permeability reduction. Heating increases the magnitude of the mineral surface charge, whereas salinity reduction increases the range over which the surface charge acts. Flow-through experiments in Berea sandstone samples indicated differences between the effect of temperature and salinity on permeability. A permeability reduction at 20°C due to salinity reduction was not reversed by restoring the salinity; a permeability reduction due to heating to 80°C was reversible by restoring the temperature to 20°C. A reversible permeability increase with increasing flow rate was observed at 80°C, but not at 20°C. Therefore, it was suggested that mobilised kaolinite particles affect permeability by a different mechanism at 80°C than at 20°C; at 80°C the main effect might be due to an alteration of pore fluid rheology, whereas at 20°C particles might be filtered in pore constrictions. DLVO theory (Derjaguin and Landau (1941); Verwey and Overbeek (1948)) was used to compare effects of temperature and salinity on surface interaction forces.

Quantitative analysis of images, in which mineralogy was mapped based on backscatter electron intensity in combination with energy dispersive X-ray analysis by using the QEMSCAN® system, was used to compare a tested sample to an untested Berea sandstone sample. During the experiment, in which an 80°C NaCl solution was injected for 150 days, apparently siderite dissolutions released iron, which was oxidised and precipitated as iron hydroxides. Lamination appears to be enhanced by precipitation of iron hydroxides predominantly in finer grained, lower porosity, lamina. The effect of enhanced lamination, as estimated based on the specific interface to the pore from image analysis, was negligible; accordingly, the experimentally measured permeability at the end of the test was only 20% lower than at the start of the test.

This investigation indicates that clay morphology and abundance has a strong effect on: the fraction of the porosity that is effective for permeability, the difference between brine and gas permeability, and the effect of temperature. Hot water injection might induce clay particle mobilisation and permeability reduction. Heating increases the magnitude of the mineral surface charge, whereas salinity reduction increases the range over which the surface charge acts. Flow-through experiments in Berea sandstone samples indicated differences between the effect of temperature and salinity on permeability. A permeability reduction at 20°C due to salinity reduction was not reversed by restoring the salinity; a permeability reduction due to heating to 80°C was reversible by restoring the temperature to 20°C. A reversible permeability increase with increasing flow rate was observed at 80°C, but not at 20°C. Therefore, it was suggested that mobilised kaolinite particles affect permeability by a different mechanism at 80°C than at 20°C; at 80°C the main effect might be due to an alteration of pore fluid rheology, whereas at 20°C particles might be filtered in pore constrictions. DLVO theory (Derjaguin and Landau (1941); Verwey and Overbeek (1948)) was used to compare effects of temperature and salinity on surface interaction forces. Quantitative analysis of images, in which mineralogy was mapped based on backscatter electron intensity in combination with energy dispersive X-ray analysis by using the QEMSCAN® system, was used to compare a tested sample to an untested Berea sandstone sample. During the experiment, in which an 80°C NaCl solution was injected for 150 days, apparently siderite dissolutions released iron, which was oxidised and precipitated as iron hydroxides. Lamination appears to be enhanced by precipitation of iron hydroxides predominantly in finer grained, lower porosity, lamina. The effect of enhanced lamination, as estimated based on the specific interface to the pore from image analysis, was negligible; accordingly, the experimentally measured permeability at the end of the test was only 20% lower than at the start of the test.

This investigation indicates that clay morphology and abundance has a strong effect on: the fraction of the porosity that is effective for permeability, the difference between brine and gas permeability, and the effect of temperature. Hot water injection might induce clay particle mobilisation and permeability reduction; however, these effects would depend on the mineralogy and pore fluid composition. Therefore, results from one formation cannot directly be generalised to other formations.

**General information**

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Organisations: Department of Civil Engineering, Section for Geotechnics and Geology, Center for Energy Resources Engineering, Geological Survey of Denmark and Greenland
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**Effects of fillers on the properties of liquid silicone rubbers (LSRs)**

Dielectric electro active polymers (DEAPs) change their shape and size under a high voltage or reversibly generate a high voltage when deformed [1,2]. One prominent method to make DEAPs performances more efficient is by adding suitable fillers [3,4]. Liquid silicone rubbers (LSRs) have relatively low viscosities, which is favorable for loading of inorganic fillers [5]. In this study, commercially available fillers, such as fumed silica (SiO2), titanium dioxide (TiO2), barium titanate (BaTiO3), copper calcium titanate (CaCu3Ti4O12, CCTO), multi-walled carbon nanotubes (MWCNTs) were added into the LSRs. The filled elastomers have both favorable properties and shortcomings. The results indicate that the hydrophobic rutile TiO2 nanofiller is a good candidate for achieving higher permittivity and breakdown, as well as favorable elastic modulus of the elastomers.
Effects of fillers on the properties of liquid silicone rubbers (LSRs)

Dielectric electro active polymers (DEAPs) change their shape and size under a high voltage or reversibly generate a high voltage when deformed. To make their performances more efficient, certain properties of the polymers like their dielectric permittivity, electrical breakdown and Young's modulus have to be modified according to the specifications of their respective applications. One such prominent method of modifying the properties is by adding suitable fillers. Liquid silicone rubbers (LSRs) have relatively low viscosities when compared with thermoplastics, which is favorable for loading of inorganic fillers. The property improvement of the filled LSRs depends on filler concentration, filler morphology, such as particle size and structure, the degree of dispersion and orientation in the matrix, and also the degree of adhesion with the polymer chains, as well as the properties of the inorganic fillers.

In this study commercially available fillers, such as fumed silica (SiO2), titanium dioxide (TiO2), barium titanate (BaTiO3), copper calcium titanate (CaCu3Ti4O12, CCTO), multi-walled carbon nanotubes (MWCNTs) were added into the LSRs and we examined how the properties of the networks were modified. The filled elastomers have both favorable properties and shortcomings. The shortcomings are of various types. Fumed silica reinforces the networks with no increase in permittivity (εr,SiO2 ~ 3.9). Barium titanate possesses high dielectric constant (εr,BaTiO3 ~ 150) but its heavy density (6.08 g/mL) deteriorates the lightweight advantage of the DEAPs. Micron-sized giant dielectric constant CCTO (εr,CCTO ~ 10000) decreases the mechanical performances of the composites. The inhomogeneous compatibility of the unmodified MWCNTs in the silicone system causes the risk of electric conductivity. Among these additives, the use of multiple titanium dioxides as filler potentially suits to special applications. In the present study, a series of TiO2 fillers were blended into LSRs, such as hydrophilic/ hydrophobic, micro/ nano scale, anatase/ rutile crystal, sphere/ core-shell structure. The results indicate that the hydrophobic rutile TiO2 nanofiller is a good candidate for achieving higher permittivity and breakdown strength, as well as favorable elastic modulus of the prepared elastomers.

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Elastic deformation behaviour of Palaeogene clay from Fehmarn Belt area

Palaeogene clay samples were obtained by high quality boring and sampling techniques (Geobore S-system), during the extensive site investigations for building a bridge in the Fehmarn Belt area to link between Rødbyhavn in Denmark and Puttgarden in Germany. The Palaeogene clay is rich in smectite and of high to very high plasticity. Comprehensive and advanced laboratory tests were done by Fugro-McClelland (in Netherlands) and by Danish Geotechnical Institute (in Denmark) on Palaeogene clays. Some of their data are included in this study. Ten Palaeogene clay samples were selected and used in this study.

Results of odometer tests done by Jessen et al. (2011) show that when Palaeogene clay is mounted in an odometer cell without access to water and loaded to its in-situ vertical effective stress and then saturated with its native salt water, the clay absorbs water and swells. This behaviour indicates that the Palaeogene clay in nature should expand at its mean effective in-situ stress. A study by Krogsbøll et al. (2012) provides some important clues about the deformation behaviour during unloading and swelling of the Palaeogene clay. In this study, we mainly focused on the elastic properties of the Palaeogene clays. Elastic wave velocities are influenced by the elastic stiffness and the density of a material. We used geotechnical and elastic wave velocity data to model the elasticity and then to relate it to mineralogy and BET surface area. We measured the mineralogy, BET surface area, bulk density, porosity, water content and saturation, elastic wave velocities, electrical resistivity and strain caused by mechanical loading. They were used together to interpret the geotechnical data. We aimed to see which physical property is a main controlling factor for the elasticity of the studied Palaeogene clay and whether we can explain the deformation behaviour from elasticity alone.

Encapsulated PDMS microspheres with reactive handles

Cured poly(dimethyl siloxane) microspheres are prepared by an emulsion polymerization reaction of silicone droplets in a continuous aqueous phase. The commonly used PDMS elastomer, Sylgard 184 from Dow Corning, is used as the dispersed phase. PDMS is polymerized and cross-linked by reacting vinyl end-terminated poly(dimethyl siloxane) oligomers with dimethylmethylhydrogen siloxane cross-linkers via the hydrosilylation reaction using platinum catalyst and heat. Weight ratios of 10:1, 20:1, and 25:1 of the PDMS mixtures are used and emulsified in water using two water-soluble surfactants as stabilizers (sodium dodecyl sulphate and polyvinylalcohol). The temperature is subsequently increased to accelerate the rate of cross-linking and prevent the prepolymer droplets from coalescing. The particle size distribution of cured PDMS microspheres is determined by Mastersizer (laser diffraction). Finally, cured PDMS microspheres are coated with poly(methyl methacrylate) using a chemical process (solvent evaporation technique). Three solvents are used in three different experiments: dichloromethane, tetrahydrofuran, and acetone. The composition and morphology of the cured PDMS microspheres and PMMA coated cured PDMS microspheres are characterized by differential scanning calorimetry, Fourier transform infrared spectroscopy in attenuated-total-reflection mode, optical microscopy, and thermogravimetric analysis. Curing profiles of PDMS elastomer with different ratios between the silicone elastomer base and the silicone elastomer curing agent are obtained. The reactivity of cured PDMS microspheres and PMMA coated cured PDMS microspheres are measured by rheology to evaluate the efficiency of the PMMA coating. © 2014 WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim.
Enzymatically Assisted CO$_2$ Removal from Flue-Gas

The enzyme carbonic anhydrase is an enzyme known to enhance CO$_2$ absorption rates. However, for economic viability in enzyme-based absorption technology, long-term stability under process-relevant conditions is needed. Thus, here enzyme stability for extended times are investigated with respect to pH, temperature, and solvent. Temperatures and pH stability were tested for up to 100 hours incubation and the enzyme was temperature stable up to 60 °C and in the pH range from 7 to 11, with some residual activity between pH 5 and 12. Furthermore, enzyme stability was tested for 7 different capture solvents for 150 days, at 1 M or 3 M solvent concentrations, 40 °C, and pH between 8-9 and 10. Residual activity was found with all samples ranging from 12 to 91% of the initial activity. This study shows that this enzyme can indeed be used for extended periods in process-relevant conditions, and thus shows promise for industrial implementation as a catalyst in carbon capture.
Equilibrium Solubility of CO₂ in Alkanolamines

Equilibrium solubility of CO₂ were measured in aqueous solutions of Monoethanolamine (MEA) and N,N-diethylethanolamine (DEEA). Equilibrium cells are generally used for these measurements. In this study, the equilibrium data were measured from the calorimetry. For this purpose a reaction calorimeter (model CPA 122 from ChemiSens AB, Sweden) was used. The advantage of this method is being the measurement of both heats of absorption and equilibrium solubility data of CO₂ at the same time. The measurements were performed for 30 mass % MEA and 5M DEEA solutions as a function of CO₂ loading at three different temperatures 40, 80 and 120 ºC. The measured 30 mass % MEA and 5M DEEA data were compared with the literature data obtained from different equilibrium cells which validated the use of calorimeters for equilibrium solubility measurements.
Equilibrium Total Pressure and CO2 Solubility in Binary and Ternary Aqueous Solutions of 2-(Diethylamino)ethanol (DEEA) and 3-(Methylamino)propylamine (MAPA)

Equilibrium total pressures were measured and equilibrium CO2 partial pressures were calculated from the measured total pressure data in binary and ternary aqueous solutions of 2-(diethylamino)ethanol (DEEA) and 3-(methylamino)propylamine (MAPA). The measurements were carried out in a commercially available calorimeter used as an equilibrium cell. The examined systems were the binary aqueous solutions of 5 M DEEA, 2 M MAPA, and 1 M MAPA and the ternary aqueous mixtures of 5 M DEEA + 2 M MAPA (5D2M) and 5 M DEEA + 1 M MAPA (5D1M), which gave liquid–liquid phase split upon CO2 absorption. The total pressures were measured and the CO2 partial pressures were calculated as a function of CO2 loading at three different temperatures 40 °C, 80 °C, and 120 °C. All experiments were reproduced with good repeatability. The measurements were carried out for 30 mass % MEA solutions to validate the experimental method. All the measured data were also compared with the results of 30 mass % MEA as a reference case. 5 M DEEA has shown high cyclic capacity. Both 2 M and 1 M MAPA showed high loading capacities at 40 °C and 120 °C. The aqueous amine mixtures, 5D2M and 5D1M, gave fairly good cyclic capacities and their results depend on the concentration of the promoter (MAPA) in the mixture. Approximate enthalpies of absorption of CO2 in all the tested aqueous amine systems were estimated from the CO2 solubility data. The measured total pressure and the estimated CO2 solubility data can be useful in thermodynamic modeling of the capture systems when aqueous DEEA–MAPA solutions are used as capture solvents.

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Experimental Study of Bacterial Penetration into Chalk Rock: Mechanisms and Effect on Permeability

Bacterial selective plugging is one of the mechanisms through which microorganisms can be applied for enhanced oil recovery, as bacteria can plug the water-swept zones of a reservoir, thus altering the flow paths and improving sweep efficiency. However, complete understanding of the penetration behavior of bacteria is lacking, especially in chalk formations where characteristic pore throat sizes are comparable with the sizes of bacterial cells. In this study, two bacterial strains, Bacillus licheniformis 421 (spore-forming) and Pseudomonas putida K12 (non-spore forming) were used to investigate the penetration of bacteria into chalk and its effect on permeability reduction. The core plugs were produced from Stevns Klint outcrop with low permeability (2–4 mD) and with pore sizes comparable to bacterial sizes. Both types of bacteria were able to penetrate and to be transported through the cores to some extent. A significantly higher number of B. licheniformis 421 was detected in the effluents as compared to P. putida K12. It was demonstrated that the spore-forming B. licheniformis 421 penetrates in the form of spores. P. putida K12 is found to penetrate the core, however, in smaller numbers compared to B. licheniformis. It was shown that both bacteria, under different injection concentrations, were capable of plugging the porous rock, as indicated by reduction of the core permeability. An incubation period of 12 days did not allow the permeability to return to initial condition. Based on the results it can be concluded that, when injected into chalk, spore forming bacteria have higher chance to survive and penetrate into deeper formation; and both types of bacteria may cause permeability reduction.

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Filled liquid silicone rubbers: Possibilities and challenges

Liquid silicone rubbers (LSRs) have been shown to possess very favorable properties as dielectric electroactive polymers due to their very high breakdown strengths (up to 170 V/μm) combined with their fast response, relatively high tear strength, acceptable Young’s modulus as well as they can be filled with permittivity enhancing fillers. However, LSRs possess large viscosity, especially when additional fillers are added. Therefore both mixing and coating of the required thin films become difficult. The solution so far has been to use solvent to dilute the reaction mixture in order both to ensure better particle dispersion as well as following for film formation properties. We show that the mechanical properties of the films as well as the electrical breakdown strength can be affected, and that the control of the amount of solvent throughout the coating process is essential for solvent borne processes. Another problem encountered when adding solvent to the highly filled reaction mixture is the loss of tension in the material upon large deformations. These losses are shown to be irreversible and happen within the first large-strain cycle.

High-performance small-scale solvers for linear Model Predictive Control

In Model Predictive Control (MPC), an optimization problem needs to be solved at each sampling time, and this has traditionally limited use of MPC to systems with slow dynamic. In recent years, there has been an increasing interest in the area of fast small-scale solvers for linear MPC, with the two main research areas of explicit MPC and tailored on-line MPC. State-of-the-art solvers in this second class can outperform optimized linear-algebra libraries (BLAS) only for very small problems, and do not explicitly exploit the hardware capabilities, relying on compilers for that. This approach can attain only a small fraction of the peak performance on modern processors. In our paper, we combine high-performance computing techniques with tailored solvers for MPC, and use the specific instruction sets of the target architectures. The resulting software (called HPMPC) can solve linear MPC problems 2 to 8 times faster than the current state-of-the-art solver for this class of problems, and the high-performance is maintained for MPC problems with up to a few hundred states.
History Matching Through a Smooth Formulation of Multiple-Point Statistics

We propose a smooth formulation of multiple-point statistics that enables us to solve inverse problems using gradient-based optimization techniques. We introduce a differentiable function that quantifies the mismatch between multiple-point statistics of a training image and of a given model. We show that, by minimizing this function, any continuous image can be gradually transformed into an image that honors the multiple-point statistics of the discrete training image. The solution to an inverse problem is then found by minimizing the sum of two mismatches: the mismatch with data and the mismatch with multiple-point statistics. As a result, in the framework of the Bayesian approach, such a solution belongs to a high posterior region. The methodology, while applicable to any inverse problem with a training-image-based prior, is especially beneficial for problems which require expensive forward simulations, as, for instance, history matching. We demonstrate the applicability of the method on a two-dimensional history matching problem. Starting from different initial models we obtain an ensemble of solutions fitting the data and prior information defined by the training image. At the end we propose a closed form expression for calculating the prior probabilities using the theory of multinomial distributions, that allows us to rank the history-matched models in accordance with their relative posterior probabilities. © 2014 The Author(s).
History Matching with Geostatistical Prior: A Smooth Formulation

We present a new method for solving the history matching problem by gradient-based optimization within a probabilistic framework. The focus is on minimizing the number of forward simulations and conserving geological realism of the solutions. Geological a priori information is taken into account by means of multipoint statistics borrowed from training images. Then production data and prior information are integrated into a single differentiable objective function, minimizer of which has a high posterior value. Solving the proposed optimization problem for an ensemble of different starting models, we obtain a set of solutions honouring both data and prior information.

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Hydrate phase equilibria of CO2+N2+aqueous solution of THF, TBAB or TBAF system

We report hydrate dissociation conditions of CO2 (15 and 30mol%)+N2 (85 and 70mol%) in the presence of aqueous solutions of THF, TBAB or TBAF. The concentrations of TBAB and TBAF in the aqueous solutions are 5wt% and 9wt% while THF concentration in aqueous solution is 3mol%. Two different experimental techniques including isochoric pressure search method and a DSC method are used to measure the hydrate dissociation conditions. A comparison is finally made with the literature data. It is expected that this study provides better understanding of hydrate phase equilibria associated with CO2 capture. © 2014 Elsevier Ltd.
Improving GC-PPC-SAFT equation of state for LLE of hydrocarbons and oxygenated compounds with water

The GC-PPC-SAFT model has been shown to be useful for predicting the liquid-liquid phase split with water [Nguyen-Huynh et al. Ind. Eng. Chem. Res. 50 (2011) 7467-7483]. In order to extend the use of this model to oxygenated compounds for a large number of families (aliphatic ethers, aldehydes, ketones, formates, acetates, propionates/butyrates, n-aliphatic acids), it is proposed to consider cross-association in addition to a binary interaction parameter \( l_{ij} \) on the combining rules for the cross-segment diameter between water and the investigated compound. The binary interaction parameters \( l_{ij} \), \( u_{ij} \), and \( w_{ij} \) are fitted on mutual solubilities of water and organic compounds. The regressed values which are obtained for each chemical family, are subsequently used for predicting infinite dilution activity coefficient in water and n-octanol/water partition coefficient.

In general, the results obtained are very much improved compared to the predictive approach discussed previously [Nguyen et al. Ind. Eng. Chem. Res. 52 (2013) 7014-7029]. The global deviation values on the decimal log scale for infinite dilution activity coefficient in water, water solubility and n-octanol/water partition coefficient are 0.377, 0.419, and 0.469, respectively. © 2014 Elsevier B.V.
Improving the Pattern Reproducibility of Multiple-Point-Based Prior Models Using Frequency Matching

Some multiple-point-based sampling algorithms, such as the snesim algorithm, rely on sequential simulation. The conditional probability distributions that are used for the simulation are based on statistics of multiple-point data events obtained from a training image. During the simulation, data events with zero probability in the training image statistics may occur. This is handled by pruning the set of conditioning data until an event with non-zero probability is found. The resulting probability distribution sampled by such algorithms is a pruned mixture model. The pruning strategy leads to a
probability distribution that lacks some of the information provided by the multiple-point statistics from the training image, which reduces the reproducibility of the training image patterns in the outcome realizations. When pruned mixture models are used as prior models for inverse problems, local re-simulations are performed to obtain perturbed realizations. Consequently, these local re-simulations lead to additional pruning in the set of conditioning data, which further deteriorates the pattern reproduction. To mitigate this problem, it is here suggested to combine the pruned mixture model with a frequency matching model. The multiple-point statistics of outcome realizations from this combined model has improved degree of match with the statistics from the training image. An efficient algorithm that samples this combined model is suggested. Finally, a tomographic cross-borehole inverse problem with prior information expressed by the combined (prior) model is used to demonstrate the effect of pattern reproducibility on the resolution of an inverse problem.

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Inhibition of Gas Hydrate Nucleation and Growth: Efficacy of an Antifreeze Protein from the Longhorn Beetle Rhagium mordax

Antifreeze proteins (AFPs) are characterized by their ability to protect organisms from subfreezing temperatures by preventing tiny ice crystals in solution from growing as the solution is cooled below its freezing temperature. This inhibition of ice growth is called antifreeze activity, and in particular, certain insect AFPs show very high antifreeze activity. Recent studies have shown AFPs to be promising candidates as green and environmentally benign inhibitors for gas hydrate formation. Here we show that an insect antifreeze protein from the longhorn beetle, Rhagium mordax (RmAFP1), the most potent protein yet found for freezing inhibition, can inhibit methane hydrates as effectively as the synthetic polymeric inhibitor polyvinylpyrrolidone (PVP). In high pressure rocking cell experiments, onset hydrate nucleation temperatures and growth profiles showed repeatable results. RmAFP1 clearly showed inhibition of hydrates compared to amino acids (l-valine and l-threonine) and the protein bovine serum albumin (BSA). This indicates that proteins or amino acids do not generally inhibit hydrate formation. The promising performance of RmAFP1 as a new green kinetic hydrate inhibitor could further the development and increased production of green hydrate inhibitors.
This paper presents an algorithm, based on the alternating direction method of multipliers, for the convex optimal control problem arising in input-constrained model predictive control. We develop an efficient implementation of the algorithm for the extended linear quadratic control problem (LQCP) with input and input-rate limits. The algorithm alternates between solving an extended LQCP and a highly structured quadratic program. These quadratic programs are solved using a Riccati iteration procedure, and a structure-exploiting interior-point method, respectively. The computational cost per iteration is quadratic in the dimensions of the controlled system, and linear in the length of the prediction horizon. Simulations show that the approach proposed in this paper is more than an order of magnitude faster than several state-of-the-art quadratic programming algorithms, and that the difference in computation time grows with the problem size. We improve the method further using a warm-start procedure.

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Measurement and Modelling of Phase Equilibrium of Oil - Water - Polar Chemicals

As the exploitable resources decrease, more sophisticated recovery methods are employed in the oil industry to produce the remaining resources. A result of using more sophisticated recovery methods is that oil field chemicals are more widely used, especially in the offshore oil production. These chemicals belong to different families like alcohols, glycols, alkanolamines, surfactants and polymers. They have various functions, e.g., methanol and MEG are used as gas hydrate inhibitors, surfactants are used to lower interfacial tension between crude oil and microemulsion and polymers in a polymer-waterflooding process act primarily as thickeners.

The main purpose of this work, focusing on the phase equilibrium of complex systems containing thermodynamic gas hydrate inhibitors, is to give a solid contribution in bridging the existing gaps in what experimental data is concerned. This was achieved not just with the measurement of new experimental data, but through the development of new experimental equipment for the study of multi-phase equilibrium. In addition to measurement of well-defined systems, LLE have been measured for North Sea oils with MEG and water.

The work can be split up into two parts:
- **Experimental**: VLE, LLE and VLLE
- **Modeling**: Well-defined systems, oil systems

In the first part, an existing experimental set-up is described and the investigation of limitations and optimizations needed for optimal use. A complete description of the equipment is made, and the results obtained in the study of reference systems presented, confirming the quality of the equipment. The equipment is used for measurement of VLE for several systems of interest: methane + water, methane + methanol, methane + methanol + water and methane + MEG.

Details dealing with the design, assembling and testing of new experimental equipment for measuring VLLE are given in chapter 3. A general insight on the processes behind the development of new equipment is given, followed by the complete description of the set-up developed in this work. The results obtained in the study of reference systems are also presented, confirming the viability of the equipment and its potential for the attainment of high quality data. Measurements were performed for VLLE of a multicomponent system consisting of methane + n-hexane + methanol + water.

In order to develop a thermodynamic model for the distribution of chemicals in oil-water systems, experimental data are required, but such data with oil systems are very rare in the literature. In this project experimental work has been carried out at Statoil R&D and an experimental method has been established and tested for such measurements. The mutual solubility of two North Sea oils, MEG and water has been measured in the temperature range of 303-323 K at atmospheric pressure.

In the second part of this work, the CPA EoS has been used for modeling hydrocarbon systems containing polar chemicals, such as water and gas hydrate inhibitor MEG or methanol. All the experimental data measured in this work have been investigated using CPA, with satisfactory results. A single temperature independent kij between the components present in the system, is usually enough to describe the solubility of all phases. Accurate predictions are made for VLLE of a quaternary system of methane + n-hexane + methanol + water, using the CPA EoS with binary interaction parameters taken from binary systems. Predictions are in good agreement with the experimental data, even for very low solubility, such as n-hexane in aqueous phase. In conclusion, the CPA EoS predicts satisfactorily the multiphase equilibrium of multicomponent water – alcohol– aliphatic hydrocarbon systems, based solely on the binary interaction parameters taken from binary systems, using the 2B association scheme for methanol and the 4C association scheme for water.

Finally, CPA has been extended to reservoir-fluid + MEG and reservoir-fluid + MEG + watersystems. The reservoir fluid consists of three condensates and four oils from fields in the North Sea. The mutual solubility of oil and MEG is satisfactorily correlated using correlations for estimating kij, for all MEG-HC pairs. Similarly the mutual solubility of condensate/oil, MEG and water is predicted satisfactorily using correlations for kij, of all MEG-HC pairs and water-HC pairs, as a function of molecular weight. The experimental trends in mutual solubility as a function of temperature and MEG content in polar phase are predicted satisfactorily which are correct in order of magnitude according to the industrial requirements.

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Measuring and modelling of the combined thermodynamic promoting effect of tetrahydrofuran and cyclopentane on carbon dioxide hydrates

This work documents both experimental data, and by thermodynamic modelling, the synergistic effect occurring in promoted carbon dioxide hydrate systems at the simultaneous presence of tetrahydrofuran and cyclopentane. Cyclopentane has previously been considered a reference among gas hydrate promoters due to its significant pressure reducing effect in hydrate forming systems such as those related to carbon dioxide capture. The present work shows that hydrate dissociation pressures may be lowered by up to 22% compared to those of the cyclopentane promoted carbon dioxide hydrate system by addition of tetrahydrofuran to the aqueous phase. It is shown experimentally that addition of approximately 5 mol% tetrahydrofuran to the aqueous phase of the cyclopentane promoted system, reduces hydrate formation pressures by approximately 20% compared to those of the cyclopentane promoted system at similar temperatures. A thermodynamic model, based on the van der Waals–Platteeuw model and the cubic-plus-association equation of state is applied to model the mixed promoter system. The model accurately predicts the data measured in this work. Furthermore, the model explains the synergistic effect by the fact that tetrahydrofuran displaces cyclopentane from the large cavities of the sII hydrate structure. The most pronounced synergistic effect (largest pressure reduction) is predicted at scenarios, where approximately half of the cyclopentane in the hydrate phase has been substituted with tetrahydrofuran. The model predicts the maximum pressure reduction compared to the cyclopentane promoted system to be approximately 22%. This happens at tetrahydrofuran concentrations of approximately 2.8–3.1 mol% in the aqueous phase, depending on the system temperature.

General information
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Organisations: Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering, CERE – Center for Energy Resources Engineering, CAPEC-PROCESS
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Measuring and Thermodynamic Modeling of De-Mixing CO2 Capture Systems

General information

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Silicone elastomers are used as dielectric electroactive polymers for making actuators, generators, sensors, and as artificial muscles in medical applications. Current requirements in the actuator manufacturing put a strict limitation on the thickness of the elastomers, such that a maximum permissible thickness is around 25–50 µm. The relatively small Young's modulus for these elastomers is a requirement for actuation capabilities. However, peeling and release of such films during manufacture processes are very difficult. To ease the release of the films, techniques such as the use of release agents like surfactants and detergents, incorporating resins in the silicone matrix and grafting/adding low surface energy functionalities to the silicone elastomer have been tested. The methods used are required not to interfere with the Young's modulus and the dielectric permittivity in a negative way. Polysorbate-20, a non-ionic surfactant, fulfills all requirements and gives the lowest peel forces for the films.

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Scopus rating (2016): SJR 0.565 SNIP 0.787 CiteScore 1.9
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Web of Science (2015): Indexed yes
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Modeling of the pressure propagation due to CO₂ injection and the effect of fault permeability in a case study of the Vedsted structure, Northern Denmark

Assessing the pressure buildup in CO₂ storage sites and especially the vertical propagation is vital for evaluation of site behavior and security. Vedsted structure in the Northern part of Jylland in Denmark consists of 290m thick Gassum Formation at 2100m depth forming the primary reservoir and is sealed by the 530m thick Fjerritslev Formation which is mainly shale lithology with very low permeability. Overlying the caprock is a number of formations forming secondary reservoirs and seals including a 420m thick Chalk Group which is overlain by 20–50m Quaternary deposits. Seismic profiling of the structure shows the presence of northwest-southeast trending faults of which some originate in the upper layer of the Gassum reservoir and some reach the base Chalk Group layer. Two faults in the upper Gassum reservoir have been interpreted to be connected to the base Chalk Group. In order to evaluate potential risks associated with vertical pressure transmission via the faults through the caprock, a number of simulation cases have been run with various fault permeabilities spanning orders of magnitude to represent both the worst and best case scenarios. Fault rock permeability data were obtained from a literature study and range from 1000mD (maximum value reported from sedimentary rock environment) for the worst case scenario down to 0.001mD (sealing faults in sedimentary rock environment) for the best case scenario. The results show that after injecting 60 million tons (Mt) of CO₂ at a rate of 1.5Mt/year for 40 years, overpressure is developed in the reservoir and about 5bar is transmitted to the base Chalk Group for the 1000mD fault permeability (open fault) case, while for the 0.001mD (sealing fault) case the pressure buildup is confined within the primary caprock. The results also show that, approximately 0.3–5.0bar overpressure can be transmitted to the base Chalk Group when the fault permeability is above 1.0mD.

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Modeling Phase Equilibria for Acid Gas Mixtures using the Cubic-Plus-Association Equation of State. 3. Applications Relevant to Liquid or Supercritical CO2 Transport

The CPA (cubic-plus-association) equation of state is applied in this work to a wide range of systems of relevance to CO2 transport. Both phase equilibria and densities over extensive temperature and pressure ranges are considered. More specifically in this study we first evaluate CPA against density data for both CO2 and CO2–water and for vapor–liquid equilibrium for mixtures of CO2 with various compounds present in transport systems. In all of these cases we consider various possibilities for modeling CO2 (inert, self-associating using two-, three-, and four sites) and the possibility of cross-association with water. Finally, we evaluate the predictive performance of CPA for multicomponent CO2 mixtures in transport systems which also include water, methane, and H2S. The results are compared to both experimental data and selected other approaches from literature. The results for the multicomponent systems are predictions using parameters solely estimated from binary data. The target of this work is two-fold: to assess the performance of the model for mixtures of practical significance but also to identify the best modeling approach so that we can arrive to an “engineering approach” for applying CPA to acid gas mixtures. The overall conclusion is that CPA performs satisfactorily; the model in most cases correlates well binary data and predicts with good accuracy multicomponent vapor–liquid equilibria. Among the various approaches investigated, the best ones are when cross association of CO2 with water is accounted for or when CO2 is considered to be a self-associating molecule (with three or four sites). The final choice on the best approach requires investigating a much larger set of mixtures including also alcohols and glycols, which will be considered in future works.

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Modeling Water Containing Systems with the Simplified PC-SAFT and CPA Equations of State

Numerous studies have been presented for modeling of water containing systems with the perturbed-chain statistical associating fluid theory (PC-SAFT) equation of state (EOS), and more than 20 water parameter sets have been published with emphasis on different applications. In this work, eight of these sets and new estimated parameters with different association schemes are systematically compared on describing properties of pure water, the liquid-liquid equilibria (LLE) of water with hydrocarbons, and the vapor-liquid (VLE) and/or vapor-liquid-liquid equilibria (VLLE) of water with 1-alcohols. An interactive procedure is further proposed for including the LLE of water with hydrocarbons into the pure fluid parameter estimation. The results show that it is possible for PC-SAFT to give an accurate description of the LLE of water and hydrocarbons while retaining satisfactory accuracy for both vapor pressure and saturated liquid density of water. For the aforementioned aqueous systems, the PC-SAFT correlations using the newly developed parameters are compared with the corresponding correlations of the cubic plus association EOS. The two models show comparable results for phase equilibria, and both of them fail to describe second-order derivative properties of water, i.e., residual isochoric heat capacity and speed of sound. The ability of the models to predict the monomer (free site) fractions of saturated pure water is investigated and discussed from various aspects. The results suggest that more experimental or theoretical studies are needed.
Modelling of cyclopentane promoted gas hydrate systems for carbon dioxide capture processes

A thermodynamic model based on the Cubic-Plus-Association equation of state and the van der Waals-Platteeuw hydrate model is applied to perform a thermodynamic evaluation of gas hydrate forming systems relevant for post-combustion carbon dioxide capture. A modelling study of both fluid phase behaviour and hydrate phase behaviour is presented. Cycloalkanes ranging from cyclopropane to cyclohexane, represents a challenge for CPA, both in the description of the pure component densities and for liquid-liquid equilibrium (LLE) in the binary systems with water. It is concluded that an insufficient amount of reliable LLE data exist for the binary system of water and cyclopentane. Additional water-in-oil data in particular are desired for this system. An unpromoted hydrate-based capture process, operating isothermally at a temperature of 280 K is simulated. The minimum pressure requirement of the first stage is estimated to be 24.9 MPa. Applying three consecutive hydrate formation/dissociation stages (three-stage capture process), a carbon dioxide-rich product (97 mol%) may be delivered at a temperature of 280 K and a pressure of 3.65 MPa. A second capture process, where cyclopentane is incorporated as a thermodynamic hydrate promoter is simulated. At the presence of cyclopentane the minimum pressure requirement of the first stage (operating at 285 K) is lowered to 1.04 MPa. This process needs
four consecutive hydrate formation/dissociation stages to produce a 95. mol% carbon dioxide-rich product stream. The vapour phases in the cyclopentane promoted process contains several mole percent cyclopentane at hydrate equilibrium conditions. At temperatures below 284. K, the entire cyclopentane bulk phase evaporates completely at hydrate forming conditions (pressures below 0.55. MPa). The present study suggests the hydrate-based separation technology to be unsuitable for the specific case of post-combustion carbon dioxide capture from power station flue gases, where operating pressures should preferably remain close to atmospheric. Even though the hydrate structure becomes available at low pressure conditions (by use of thermodynamic promoters), carbon dioxide may not necessarily enter the solid phase in significant amounts. © 2014 Elsevier B.V.
Modelling of tetrahydrofuran promoted gas hydrate systems for carbon dioxide capture processes

A thermodynamic study of a novel gas hydrate based CO2 capture process is presented. The model predicts this process unsuitable for CO2 capture from power station flue gases. A thermodynamic modelling study of both fluid phase behaviour and hydrate phase behaviour is presented for the quaternary system of water, tetrahydrofuran, carbon dioxide and nitrogen. The applied model incorporates the Cubic-Plus-Association (CPA) equation of state for the fluid phase description and the van der Waals-Platteeuw hydrate model for the solid (hydrate) phase. Six binary pairs are studied for their fluid phase behaviour. CPA descriptions are adjusted when needed by correlation of binary parameters in the applied mixing- and combining rules. Kihara cell potential parameters in the hydrate model are regressed for the three hydrate formers, tetrahydrofuran, carbon dioxide and nitrogen. The developed model provides highly accurate descriptions of both fluid- and hydrate phase equilibria in the studied system and its subsystems. The developed model is applied to simulate two simplified, gas hydrate-based processes for post-combustion carbon dioxide capture from power station flue gases. The first process, an unpromoted hydrate process, operates isothermally at a temperature of 280 K. Applying three consecutive hydrate formation/dissociation stages (three-stage capture process), a carbon dioxide-rich product (97 mol%) is finally delivered at a temperature of 280 K and a pressure of 3.65 MPa. The minimum pressure requirement of the first stage is estimated to be 24.9 MPa, corresponding to the incipient hydrate dissociation pressure at 280 K for the considered flue gas. A second simulated carbon dioxide capture process uses tetrahydrofuran as a thermodynamic promoter to reduce the pressure requirements. By doing so the minimum pressure requirement of the first capture stage is lowered to 0.41 MPa. Selectivity towards carbon dioxide in the hydrate phase is however lower than in the unpromoted process. Therefore the tetrahydrofuran promoted capture process needs four consecutive hydrate formation/dissociation stages to produce a 96 mol% carbon dioxide-rich product stream. This stream is delivered at 280 K and a pressure of 0.17 MPa. The present modelling study suggests several drawbacks of using tetrahydrofuran as a thermodynamic hydrate promoter, when applied in low-pressure, hydrate-based gas separation processes. Due to the high volatility of this compound, the promoter readily transfers to the vapour phase. Furthermore, tetrahydrofuran lowers the selectivity towards carbon dioxide, and the gas uptake in general, in the hydrate phase compared to the unpromoted system. © 2014 Elsevier B.V.

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BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.227 SNIP 1.09
Web of Science (2008): Indexed yes
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Web of Science (2007): Indexed yes
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Web of Science (2006): Indexed yes
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Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 0.985 SNIP 1.349
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Scopus rating (2003): SJR 1.193 SNIP 1.301
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 0.722 SNIP 1.101
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Scopus rating (2001): SJR 0.966 SNIP 1.284
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 0.87 SNIP 0.898
Model Predictive Control for Smart Energy Systems

In this thesis, we consider control strategies for flexible distributed energy resources in the future intelligent energy system – the Smart Grid. The energy system is a large-scale complex network with many actors and objectives in different hierarchical layers. Specifically, the power system must supply electricity reliably to both residential and industrial consumers around the clock. More and more fluctuating renewable energy sources, like wind and solar, are integrated in the power system. Consequently, uncertainty in production starts to affect an otherwise controllable power production significantly. A Smart Grid calls for flexible consumers that can adjust their consumption based on the amount of green energy in the grid. This requires coordination through new large-scale control and optimization algorithms. Trading of flexibility is key to drive power consumption in a sustainable direction. In Denmark, we expect that distributed energy resources such as heat pumps, and batteries in electric vehicles will mobilize part of the needed flexibility.

Our primary objectives in the thesis were threefold:

1. Simulate the components in the power system based on simple models from literature (e.g. heat pumps, heat tanks, electrical vehicle battery charging/discharging, wind farms, power plants).

2. Embed forecasting methodologies for the weather (e.g. temperature, solar radiation), the electricity consumption, and the electricity price in a predictive control system.

3. Develop optimization algorithms for large-scale dynamic systems. This includes decentralized optimization and simulation on realistic large-scale dynamic systems.

Chapter 1 introduces the power system, the markets, and the main actors. The objectives and control hierarchy is outlined while Aggregators are introduced as new actors.

Chapter 2 provides linear dynamical models of Smart Grid units: Electric Vehicles, buildings with heat pumps, refrigeration systems, solar collectors, heat storage tanks, power plants, and wind farms. The models can be realized as discrete time state space models that fit into a predictive control system.

Chapter 3 introduces Model Predictive Control (MPC) including state estimation, filtering and prediction for linear models.

Chapter 4 simulates the models from Chapter 2 with the certainty equivalent MPC from Chapter 3. An economic MPC minimizes the costs of consumption based on real electricity prices that determined the flexibility of the units. A predictive control system easily handles constraints, e.g. limitations in power consumption, and predicts the future behavior of a unit by integrating predictions of electricity prices, consumption, and weather variables. The simulations demonstrate the expected load shifting capabilities of the units that adapts to the given price predictions. We furthermore evaluated control performance in terms of economic savings for different control strategies and forecasts.

Chapter 5 describes and compares the proposed large-scale Aggregator control strategies. Aggregators are assumed to play an important role in the future Smart Grid and coordinate a large portfolio of units. The developed economic MPC controllers interfaces each unit directly to an Aggregator. We developed several MPC-based aggregation strategies that coordinates the global behavior of a portfolio of units by solving a large-scale optimization and control problem. We applied decomposition methods based on convex optimization, such as dual decomposition and operator splitting, and developed price-based aggregator strategies.

Chapter 6 provides conclusions, contributions and future work.

The main scientific contributions can be summarized to:

• Linear dynamical models of flexible Smart Grid units: heat pumps in buildings, heat storage tanks, and electric vehicle batteries.
• Economic MPC that integrates forecasts in the control of these flexible units.
• Large-scale distributed control strategies based on economic MPC, convex optimization, and decomposition methods.
Monolithic growth of partly cured polydimethylsiloxane thin film layers
The demand for monolithic structures in many applications has increased to enable more reliable and optimized performances such as for dielectric electroactive polymers (DEAPs). For the layers of the elements to grow efficiently together, it is first of all required that the layers adhere together to enable interlayer crosslinking reactions either by application of an adhesion promoter or by ensuring that there are reactive, complementary sites available on the two surfaces. Polydimethylsiloxane (PDMS) is a widely used polymer for DEAPs. In this work, two-layered PDMS films are adhered together at different curing times. The monolithic films are investigated by rheology, scanning electron microscope, mechanical testing, dielectric relaxation spectroscopy, thermal gravimetric analysis (TGA) and differential scanning calorimetry (DSC). The morphology, mechanical and dielectric properties, as well as thermal stabilities of the bilayer elastomer films are observed to change with the curing time of the monolayers before lamination. The objective of this work is to create adhesion of two layers without destroying the original viscoelastic properties of the PDMS films, and hence enable, for example, adhesion of two microstructured films which is currently a crucial step in the large-scale production of DEAPs. © 2014 The Society of Polymer Science, Japan (SPSJ) All rights reserved.
Multi-dimensional population balance models of crystallization processes

A generic and model-based framework for batch cooling crystallization operations has been extended to incorporate continuous and fed-batch processes. Modules for the framework have been developed, including a module for reactions, allowing the study of reactive crystallization within the framework. A kinetic model library together with an ontology for knowledge representation has been developed, in which kinetic models and relations from the literature are stored along with the references and data. The model library connects to the generic modelling framework as well, as models can be retrieved, analyzed, used for simulation and stored again. The model library facilitates comparison of expressions for kinetic phenomena and is tightly integrated with the model analysis tools of the framework. Through the framework, a model for a crystallization operation may be systematically generated and parameters for the simulation can be found in the database. A procedure for parameter estimation has been illustrated based on experimental work. The identifiability of the models has been discussed in relation to parameter estimation using sensitivity analysis. Some important identifiability issues have been investigated using the model structure to simulate perfect data and data with white noise added to it. It is found that the kinetic models may not be reliably estimated from the concentration profile using the parameter estimation procedure for both perfect and noisy data. The framework has been applied to case studies involving inorganic and organic compounds, including an active pharmaceutical ingredient (paracetamol) crystallized from different solvents. The case studies have been used to demonstrate the versatility of the framework.
Negative Flash for Calculating the Intersecting Key Tie lines in Multicomponent Gas Injection

Gas injection is a widely used enhanced oil recovery method, and its application is expected to increase in the foreseeable future. In order to build a method of characteristics solution to a two-phase gas injection system, we must construct the composition route from the injection gas to the initial oil where all the intersecting key tie lines must be identified. Calculation of these intersecting tie lines requires a series of special negative flashes, which allow not only phase fractions outside the physical interval $[0,1]$ but also negative feed compositions. The phase compositions from one negative flash are used to recombine the feed for the next negative flash. Despite the apparent complexity due to multicomponent phase equilibrium and transport, for pure component gas injection, negative flash and elimination of components can be performed in an alternating manner. In particular, if K-values are constant, there exists a simple feature that the vapor fraction roots (beta-roots) for the RachfordRice equation for the initial oil are the roots to be found in all the negative flashes involved. This leads to a simple and well-structured algorithm for the solution with constant K-values. A special problem with pure component gas injection is that there could be two possible roots in the beta-interval of interest. But if the component to be eliminated is left with an infinitesimal amount due to the diffusion or dispersion effects, only the larger root can still give non-negative phase compositions and should thus be selected. For multicomponent gas injection with constant K-values, the vapor fraction roots in all the involved negative flashes are simply from the vapor fraction roots for the initial oil (beta-roots) and those for the injection gas (lambda-roots). By solving just two negative flashes for the initial oil and the injection gas and using proper selection sequences for these beta- and lambda-roots, we can readily determine all the intersecting tie lines for constant K-values.

General information

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BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.012 SNIP 1.292 CiteScore 2.85
Web of Science (2014): Indexed yes
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Scopus rating (2013): SJR 0.982 SNIP 1.243 CiteScore 2.6
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Novel encapsulation technique for incorporation of high permittivity fillers into silicone elastomers

The research on soft elastomers with high dielectric permittivity for the use as dielectric electroactive polymers (DEAP) has grown substantially within the last decade. The approaches to enhance the dielectric permittivity can be categorized into three main classes: 1) Mixing or blending in high permittivity fillers, 2) Grafting of high permittivity molecules onto the polymer backbone in the elastomer, and 3) Encapsulation of high permittivity fillers. The approach investigated here is a new type of encapsulation which does not interfere with the mechanical properties to the same content as for the traditionally applied thermoplastic encapsulation. The properties of the elastomers are investigated as function of the filler content and type. The dielectric permittivity, dielectric loss, conductivity, storage modulus as well as viscous loss are compared to elastomers with the same amounts of high permittivity fillers blended into the elastomer, and it is found that the encapsulation provides a technique to enhance some of these properties.

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Novel method to prepare multiwalled carbon nanotube/poly(dimethyl siloxane) (MWCNT/PDMS) non-conducting composites

In this study a new method of carbon nanotube (CNT) incorporation was employed for the preparation of ultraviolet (UV) curable CNT filled poly (dimethyl siloxane) (PDMS) composites. The composites were designed to contain loadings of CNT above the percolation threshold without becoming conductive due to a localized distribution of CNT. Ultrasonicated and dispersed multiwalled CNTs were mixed with short chain \(^{-}\) vinyl terminated PDMS. When the whole mixture containing dispersed CNT and short chain PDMS was irradiated with UV radiation in presence of deficient amount of hexa functional thiol PDMS crosslinker and a photoinitiator, hyperbranched PDMS layer was formed over the CNTs. The prepared hyperbranched CNTs were mixed in different weight ratios (0.33%, 0.66%, 1%) with long chain \(^{-}\) vinyl terminated PDMS and crosslinked subsequently with the same hexa functional thiol PDMS via UV photoinitiated thiol-ene chemistry to obtain the networks. Rheology of the prepared networks showed a gradual decrease in storage modulus (\(G'\)) in the entire frequency range as the amount of CNT was increased due to a reduction in crosslinking density imposed by the CNT was increased due to a reduction in crosslinking density imposed by the CNTs. Dielectric spectroscopy measurements showed an increasing trend in permittivity in all the composites with increasing CNT loadings and AC conductivity measurements confirmed non-percolating behavior of the prepared composites.

On petroleum fluid characterization with the PC-SAFT equation of state

The perturbed-chain statistical associating fluid theory (PC-SAFT) equation of state has shown promising results for describing complex phase behaviors and high pressure properties of various systems. It has been proposed as an alternative to the classical cubic equations of state in the petroleum industry. It is, however, far from a simple task to develop a sophisticated oil characterization method for the PC-SAFT EOS. In this work, in order to answer some fundamental questions of developing new characterization methods for PC-SAFT, six methods are proposed to estimate the model parameters by combining the well-behaved correlations of homologous series with the PNA contents and/or by using different fitting approaches. Along with different options in characterization procedure, the performance of these methods is investigated on PVT calculations, i.e. predicting the saturation pressure and density of 80 petroleum fluids over wide temperature, pressure and composition conditions. These options include the molar composition distribution, the specific gravity correlation, the number of pseudo-components, the estimation method of PNA contents and the binary interaction parameters. Two candidate methods are showing better overall performance than the others, with deviations less than 6.0% and 1.3% of saturation pressure and density, respectively. These two methods are further studied for predicting more complete sets of PVT data, i.e. constant mass expansion, differential liberation and separator test, of three petroleum fluids. The results are promising if compared to those available in the literature. © 2014 Elsevier B.V.
On solving the Rachford-Rice equation with higher order methods

The Rachford-Rice equation calculates the amounts and compositions of two equilibrium phases at constant K-factors. This single variable equation is a perfect candidate for applying higher order iteration methods because the additional cost for evaluating the derivatives with order higher than two is relatively low. This study compares the performance of Householder's high order iterations up to order seven. In addition, a method to improve the initial estimate is proposed for the situation where the Rachford-Rice function shows abrupt change close to the asymptotes and overshooting happens. The proposed method can largely reduce repeated use of the bisection adjustment in the subsequent iterations. The comparison shows that the Householder's iteration with order three or four gives the best performance on average.

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BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.874 SNIP 0.998 CiteScore 1.99
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 0.982 SNIP 1.248 CiteScore 2.28
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.007 SNIP 1.274 CiteScore 2.31
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
On the predictive capabilities of CPA for applications in the chemical industry: Multicomponent mixtures containing methylmethacrylate, dimethyl-ether or acetic acid

The predictive performance of the CPA (Cubic-Plus-Association) equation of state for applications relevant to the chemical industry is illustrated in this work. Three such applications inspired by industrial requests/interest are illustrated here, all of which involve aqueous multicomponent mixtures exhibiting vapor-liquid (VLE) and/or liquid-liquid (LLE) equilibrium. The first two cases include mixtures of methyl-methacrylate with acetone or methanol and dimethyl-ether with ethanol, respectively. In these two cases, the classical form of CPA is used. The third case involves aqueous mixtures with acetic acid, esters, ethers and alcohols, and in this case for water-acetic acid the CPA-Huron Vidal (CPA-HV) version of the model is used. For the latter binary mixture, new CPA-HV binary parameter sets are estimated using, among others, data for activity coefficients at infinite dilutions. The modeling approach is similar in all three cases, i.e. the binary parameters are solely fitted to binary data and thus all multicomponent calculations are considered predictions. It is shown that CPA correlations for binary systems are excellent in all cases using temperature independent parameters except for the acetic acid-water system for which different parameter sets at different temperatures can be recommended. Even with the use of CPA-HV mixing rules, modeling of the acetic acid-water system with few interaction parameters remains a challenging task. Excellent simultaneous VLE and LLE correlation is obtained for complex systems such as aqueous mixtures with ethers and esters. The multicomponent results are, with a few exceptions, very satisfactory, especially for the vapor-liquid
equilibrium cases. For the demanding aqueous acetic acid-water containing systems, one parameter set is recommended at the end for modeling ternary or multicomponent mixtures containing acetic acid and water.

**General information**

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Organisations: Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering, Center for Energy Resources Engineering, Aristotle University of Thessaloniki
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Scopus rating (2016): CiteScore 2.79 SJR 0.813 SNIP 1.303
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Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.027 SNIP 1.692 CiteScore 2.91
Web of Science (2014): Indexed yes
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Scopus rating (2010): SJR 0.87 SNIP 1.317
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.742 SNIP 1.029
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.645 SNIP 0.718
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 0.572 SNIP 0.787
Scopus rating (2006): SJR 0.629 SNIP 0.823
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 0.752 SNIP 1.02
Web of Science (2005): Indexed yes
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Permeability, compressibility and porosity of Jurassic shale from the Norwegian-Danish Basin

The Fjerritslev Formation in the Norwegian-Danish Basin forms the main seal to Upper Triassic-Lower Jurassic sandstone reservoirs. In order to estimate the sealing potential and rock properties, samples from the deep wells Vedsted-1 in Jylland, and Stenlille-2 and Stenlille-5 on Sjaeland, were studied and compared to samples from Skjold Flank-1 in the Central North Sea. Mineralogical analyses based on X-ray diffractometry (XRD) show that onshore shales from the Norwegian-Danish Basin are siltier than offshore shales from the Central Graben. Illite and kaolinite dominate the clay fraction. Porosity measurements obtained using helium porosimetry-mercury immersion (HPMI), mercury injection capillary pressure (MICP) and nuclear magnetic resonance (NMR) techniques on the shale samples show that MICP porosity is 6-10% lower than HPMI or NMR porosity. Compressibility, from uniaxial loading, and elastic wave velocities were measured simultaneously on saturated samples under drained conditions at room temperature. Uniaxial loading tests indicate that shale is significantly stiffer in situ than is normally assumed in geotechnical modelling. Permeability can be predicted from elastic moduli, and from combined MICP and NMR data. The permeability predicted from Brunauer-Emmett-Teller (BET)-specific surface-area measurements using Kozeny's formulation for these shales, being rich in silt and kaolinite, falls in the same order of magnitude as permeability measured from constant rate of strain (CRS) experiments but is two-three orders of magnitude higher than the permeability predicted from the 1998 model of Yang & Aplin, which is based on clay fraction and average pore radius. When interpreting CRS data, Biot's coefficient has a significant and systematic influence on the resulting permeability of deeply buried shale.

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Organisations: Department of Civil Engineering, Section for Geotechnics and Geology, Center for Energy Resources Engineering, Vattenfall A/S, Geological Survey of Denmark and Greenland
Authors: Mbia, E. N. (Ekstern), Fabricius, I. L. (Intern), Krogsbøll, A. (Intern), Frykman, P. (Ekstern), Dalhoff, F. (Ekstern)
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Web of Science (2017): Indexed Yes
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Scopus rating (2016): SJR 0.698 SNIP 0.909 CiteScore 1.46
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.578 SNIP 0.897 CiteScore 1.39
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.877 SNIP 1.242 CiteScore 1.59
Permeability, diffusivity and solubility of carbon dioxide in fluoropolymers: An experimental and modeling study

Carbon dioxide has successfully been used as an alternative refrigerant in many applications, replacing chlorofluoro- and hydrofluorocarbons (CFCs and HFCs), due to its negligible ozone depletion and significantly lower global warming potential. However, the use of carbon dioxide as a refrigerant requires a refrigeration cycle with greater extremes of pressure, placing greater demands on the plant's seals and packings. The integrity of the refrigeration system (it should release as little refrigerant as possible to the atmosphere) depends crucially on the material used for the seals and packings. Using a high-pressure permeation cell, the permeability and diffusivity of carbon dioxide were measured in several polymers used as packing and sealing materials. These were the fluoropolymers PTFE, FKM and TFM, both pure and containing glass, graphite, Ekonol and polysulfone as additives. The solubility coefficient of carbon dioxide in these polymers was then obtained as the ratio of the measured permeability and diffusivity data. Measurements were carried out over a pressure range of 45-50 bar and a temperature range of 40-80 °C. The solubility of carbon dioxide in the polymers is then modeled with the Simplified Perturbed Chain - Statistical Associating Fluid Theory (sPC-SAFT) equation of state. Pure component parameters were determined using an extrapolation method based on the lower molecular weight monomer and available density data for the polymers. In the case of copolymers, mixing rules were used to determine parameters. Carbon dioxide solubility can be accurately correlated to the measured data with the sPC-SAFT equation of state using a temperature-independent binary interaction parameter. © Springer Science+Business Media New York (outside the USA) 2014.

General information
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Organisations: Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering, CERE – Center for Energy Ressources Engineering
Petrophysical Analysis of Siliceous-Ooze Sediments, More Basin, Norwegian Sea

Pelagic siliceous-ooze sediments occur above the hydrocarbon reservoir of the Ormen Lange gas field in More Basin, Norwegian Sea. A possible hydrocarbon prospect of siliceous ooze was proposed, but siliceous ooze is significantly different in texture from most commonly known reservoir rocks. Logging and core analysis data were integrated to characterize and evaluate these sediments. "True" density porosity was obtained by taking the number of electrons per unit volume of bulk siliceous ooze into account and it was calibrated to the overburden-corrected core porosity. A grain-density log was calculated from the gamma-ray log and empirical grain-density data were calibrated with X-ray diffraction analysis data. The grain-density log was used with the calculated true porosity log and the brine density of 1.025 g/cm(3) to convert the bulk-density log from conventional limestone and water scaling of electron density to opal and brine scaling of electron density. The neutron-porosity log was corrected for the hydrogen-index contribution of solid phase. The corrected neutron porosity is lower than the conventional neutron porosity by 3 to 4 p.u. The true density porosity and the corrected neutron porosity are similar. This indicates that our interpretation is consistent, such that it can be applied elsewhere. The studied sediments apparently do not contain hydrocarbons. The relatively low Biot's coefficient, averaging approximately 0.94, indicates that the siliceous ooze is relatively stiff. Amplitude-versus-offset analysis indicated that an oil-saturated sandstone layer can be distinguished from water-saturated siliceous ooze.
Petrophysical and rock-mechanics effects of CO2 injection for enhanced oil recovery: Experimental study on chalk from South Arne field, North Sea

Enhanced oil recovery by CO2 injection (CO2-EOR) is a tertiary oil recovery process which has a prospective for being used, at the same time, as an effective technique for carbon dioxide storage. There is a huge potential for additional oil production and CO2 storage in the North Sea depleted chalk reservoirs. North Sea chalk is characterized by high porosity but also high specific surface causing low permeability. A high porosity provides room for CO2 storage, while a high specific surface causes a high risk for chemical reaction and consequently for mechanical weakening. In order to address this issue we studied two types of chalk from South Arne field, North Sea: (1) Ekofisk Formation having >12% non-carbonate and (2) Tor Formation, which has less than 5% non-carbonate. We performed a series of laboratory experiments to reveal the changes in petrophysical and rock-mechanics properties due to the injection of CO2 at supercritical state. We analyzed these changes with respect to the differences in porosity, specific surface, pore stiffness, wettability, mineralogy and mechanical strength. We observed a 2–3% increase in porosity, a minor decrease of specific surface and consequently a small increase in permeability. A decrease in elastic stiffness is indicated by an increase of Biot's effective stress coefficient (α) by 1–2%. Nuclear Magnetic Resonance (NMR) data indicated no change in wettability and the samples remained water wet. We found that the effect of CO2 injection on both petrophysical and mechanical properties of chalk depends on carbonate content. Pure chalk with high carbonate content was found to be vulnerable to mechanical weakening due to CO2 injection, whereas, no significant mechanical effect was observed in the impure chalk of Ekofisk Formation. It should in this context be noted that the experiments spanned only 8 days, therefore long term effects cannot be ruled out. In spite of weakening of the chalk, we expect only minor mechanical effects, because the weakening also causes a lowering of effective stress due to an increase in effective stress coefficient. Extensive time-lapse monitoring strategies are required during a CO2-EOR process for the measurement of changes in reservoir properties that may cause deformation of and leakage from a reservoir. Results of this study will provide data for designing future monitoring strategies based on 4D seismic.

General information
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Organisations: Department of Civil Engineering, Section for Geotechnics and Geology, Center for Energy Resources Engineering, Danish Geotechnical Institute
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Scopus rating (2016): CiteScore 2.56 SJR 0.764 SNIP 1.631
Web of Science (2016): Indexed yes
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Scopus rating (2015): SJR 0.801 SNIP 1.652 CiteScore 2.38
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Petrophysics of Palaeogene sediments

Changes of physical properties of sedimentary rocks with increasing burial depth have implications in hydrocarbon explorations. Physical properties of buried sediment are controlled by several factors such as mineralogical composition, depositional texture and burial depth. The main theme for this Ph.D. study is petrophysics of Palaeogene sediments, aiming to gain better knowledge and understanding of the petrophysical characteristics of the studied sediments. To limit the scope, the Ph.D. study focused only on three selected lithologies: 1) the Eocene chalk of the Atlantic Ocean basins, 2) the siliceous ooze sediments from the Norwegian Sea, and 3) the Palaeogene shale from both the Atlantic and the Danish basins. The three geological settings differ in water depths, temperature, effective stress and pressure. If the factors governing physical properties of the studied lithologies are well defined and understood this would benefit various areas in petroleum industry.

The three studied lithologies are relatively soft and weak sediments, but they are economically important especially in petroleum industry. Drilling through intervals of shale or siliceous ooze sediments could result in severe and very costly borehole instability problems which are closely connected with the "bulk properties" of shale. In practice, the main technological challenge is to keep the borehole sufficiently stable until casing is set. Knowing the real in-situ effective stress is crucial to understand and to predict the geomechanical behaviour of shale. Biot's coefficient ($\beta$) for elastic deformation is an important parameter involves in the estimation of effective stress. However, engineers usually assume $\beta$...
equal to one when estimating in-situ vertical effective stress on buried sediments, but, this assumption is not always right, especially for the deep-sea cemented sediments where the water depth is high, and it may underestimate the real effective stress which may lead to severe engineering consequences such as a petroleum reservoir may suffer compaction or deformations as a result of changing in stress state during drilling operations and hydrocarbon production, or even during massive excavations for building tunnels. If the effective stress exceeds the strength of the rock, failure develops. Thus, estimating a more realistic effective stress allows determining the optimum drilling parameters to reduce problems related to borehole stability. This Ph.D. study stressed on the importance of using correct β value in estimation of vertical effective stress especially on deep-sea sediments. To assess the geomechanical stability and the stiffness of the three studied lithologies, their β was found and used to calculate the in-situ vertical effective stress.

The primary objectives of this Ph.D. study were: 1) to investigate and evaluate the influence of mineralogical composition, depositional texture and burial depth on petrophysical properties of Palaeogene sediments and to find out how the physical properties are related; 2) to know the stiffness of the studied lithologies based on their β values; and 3) to link the diagenesis of siliceous ooze with logging interpretation. The secondary goals were: to show how crucial is the use the correct value of β on estimation of vertical effective stress especially on deep-sea sediments; to establish a relationship between static and dynamic modulus of shale which could be used to estimate geotechnical drained elastic modulus from bulk density and sonic velocity.

The influence of burial depth on physical properties of Atlantic Palaeogene shale and Eocene chalk has been studied. Changes in physical properties of the Atlantic Palaeogene shale as a function of burial depth was related to the vertical effective stress and shale mineralogy. The influence of choice of β value on estimation of effective stress on deep-sea shale was shown. The obtained results could be relevant for drilling, basin analysis, seismic interpretation and hydrocarbon exploration. The diagenesis of Eocene chalk was studied. The changes of porosity and sonic velocity trends of the studied chalk were related to effective stress and time–temperature index (TTI) of thermal maturity of chalk. For each depth, effective stresses as defined by Terzaghi and by Biot were calculated. It is concluded that the use of the Biot's effective stress concept provides more realistic estimate of vertical effective stress of the studied chalk. Bottom-hole temperature data were used to calculate the TTI as defined by Lopatin. Porosity and compressional wave velocity data were correlated with effective stresses and to TTI. Based on the results, an equation to predict porosity reduction with increasing burial stress in chalk was proposed. The proposed equation is relevant for basin analysis and hydrocarbon exploration to predict porosity if sonic velocity (e.g. seismic velocity) data for subsurface chalk are available. A possible hydrocarbon prospect of the Møre Basin siliceous ooze in the Norwegian Sea has been proposed, but siliceous ooze is significantly different in texture from most commonly known hydrocarbon reservoirs. This Ph.D. study includes results of petrophysical and the amplitude versus offset (AVO) analyses of siliceous ooze. Based on fundamental relationships, ways of correcting density and neutron porosity logs were proposed. Additionally, the values of β and the AVO signature of water saturated siliceous ooze were obtained. A new approach for deriving reliable and accurate porosity of siliceous ooze is proposed here. The true density porosity was calculated by taking the number of electrons per unit volume into account. The true density porosity is similar to the corrected neutron porosity which indicates that the proposed interpretation is consistent. The proposed approach can be applied elsewhere and could be useful for petrophysics community. The studied siliceous ooze intervals apparently do not contain hydrocarbons.

X-ray diffraction (XRD) analyses and surface area by BET method have been done on 116 sediment samples collected from different geological units in the Fehmarn Belt area which is located between Denmark and Germany. Based on the XRD and BET results, ten preserved whole-core samples of the Palaeogene clay were selected and used in the laboratory testing for studying the elastic deformation properties of the naturally water saturated Palaeogene clay. Hence, this Ph.D. study presents the results of a wide characterization of Palaeogene clay. The main focus was on elastic properties which were examined and analysed in terms of mineralogical, physical and geotechnical properties. Elastic wave velocity is controlled by the elasticity and the density of a material. The deformation properties and the velocity of elastic waves were measured here simultaneously during triaxial testing under drained conditions. Geotechnical and elastic wave velocity data were used to model the elasticity and to relate it to clay mineralogy and BET. The mineralogy, BET, classification parameters, elastic wave velocities and strain caused by mechanical loading on the ten studied clay samples were measured and used together to interpret the geotechnical data and to observe the effect of mineralogy on elastic properties. The aim was to see which physical property is a main controlling factor for the elasticity of the Palaeocene clay and whether the deformation behaviour can be explained from elasticity alone. The obtained results can aid in the estimation of geotechnical drained elastic modulus from bulk density and elastic wave velocity and may have implications in engineering practice, including structural design and slope stability analysis.

**General Information**

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Porosity and sonic velocity depth trends of Eocene chalk in Atlantic Ocean: Influence of effective stress and temperature

We aimed to relate changes in porosity and sonic velocity data, measured on water-saturated Eocene chalks from 36 Ocean Drilling Program drill sites in the Atlantic Ocean, to vertical effective stress and thermal maturity. We considered only chalk of Eocene age to avoid possible influence of geological age on chalk compaction trends. For each depth, vertical effective stresses as defined by Terzaghi and by Biot were calculated. We used bottom-hole temperature data to calculate the time–temperature index of thermal maturity (TTI) as defined by Lopatin. Porosity and compressional wave velocity data were correlated to vertical effective stresses and to TTI. Our porosity data showed a broader porosity trend in the mechanical compaction zone, and the onset of the formation of limestone at a shallower burial depth than the porosity data of the Ontong Java Plateau chalk show. Our porosity data do not show or at least it is difficult to define a clear pore-stiffening contact cementation trend as the Ontong Java Plateau chalk. Mechanical compaction is the principal cause of porosity reduction (at shallow depths) in the studied Eocene chalk, at least down to about 5MPa Terzaghi's effective stress corresponding to a porosity of about 35%. This indicates that mechanical compaction is the principal agent of porosity reduction. Conversely, at deeper levels, porosity reduction is accompanied by a large increase in sonic velocity indicating pore-filling cementation. These deep changes are correlated with TTI. This indicates pore-filling cementation via an activation energy mechanism. We proposed a predictive equation for porosity reduction with burial stress. This equation is relevant for basin analysis and hydrocarbon exploration to predict porosity if sonic velocity data for subsurface chalk is available.

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Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.692 SNIP 1.751 CiteScore 1.95
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Predicting Plasma Glucose From Interstitial Glucose Observations Using Bayesian Methods

One way of constructing a control algorithm for an artificial pancreas is to identify a model capable of predicting plasma glucose (PG) from interstitial glucose (IG) observations. Stochastic differential equations (SDEs) make it possible to account both for the unknown influence of the continuous glucose monitor (CGM) and for unknown physiological influences. Combined with prior knowledge about the measurement devices, this approach can be used to obtain a robust predictive model. A stochastic-differential-equation-based gray box (SDE-GB) model is formulated on the basis of an identifiable physiological model of the glucoregulatory system for type 1 diabetes mellitus (T1DM) patients. A Bayesian method is used to estimate robust parameters from clinical data. The models are then used to predict PG from IG observations from 2 separate study occasions on the same patient. First, all statistically significant diffusion terms of the model are identified using likelihood ratio tests, yielding inclusion of $\sigma_{Isc}$, $\sigma_{Gp}$, and $\sigma_{Gsc}$. Second, estimates using maximum likelihood are obtained, but prediction capability is poor. Finally a Bayesian method is implemented. Using this method the identified models are able to predict PG using only IG observations. These predictions are assessed visually. We are also able to validate these estimates on a separate data set from the same patient. This study shows that SDE-GBs and a Bayesian method can be used to identify a reliable model for prediction of PG using IG observations obtained with a CGM. The model could eventually be used in an artificial pancreas.
Process Design of Industrial Triethylene Glycol Processes Using the Cubic-Plus-Association (CPA) Equation of State

The Cubic-Plus-Association (CPA) equation of state (EoS) has already been proven to be a successful model for phase equilibrium calculations for systems containing glycols. In the present work, we interface a thermodynamic property package (Thermo System), based on CPA, with Aspen HYSYS through the CAPE-OPEN standards. We, then, simulate certain binary and multicomponent systems where experimental data are available in the literature and which are critical for process design of natural gas dehydration units by triethylene glycol (TEG). We also demonstrate the potential of CPA for the process design of liquid-liquid extraction of aromatic hydrocarbons by TEG. Comparisons between simulation and experimental results are presented in order to illustrate the reliability of Thermo System while it is used in a process simulator for industrial applications. Detailed analysis on selecting TEG pure compound parameters and on calculating TEG-water binary parameters is shown. Missing binary interaction parameters are regressed and presented for various binary systems, and a relationship between the interaction parameters and alkane molecular weight is obtained for TEG-alkane binary systems. A simulation case study of a typical natural gas dehydration process is also presented.

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Organisations: Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering, Center for Energy Resources Engineering
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Pages: 11766-11778
Quantifying porosity, compressibility and permeability in Shale

The Fjerritslev Formation in the Norwegian-Danish Basin forms the main seal to Upper Triassic-Lower Jurassic sandstone reservoirs. In order to estimate rock properties Jurassic shale samples from deep onshore wells in Danish basin were studied. Mineralogical analysis based on X-ray diffractometry (XRD) of shale samples show about 50% silt and high content of kaolinite in the clay fraction when compared with offshore samples from the Central Graben. Porosity measurements from helium porosimetry-mercury immersion (HPMI), mercury injection capillary pressure (MICP) and nuclear magnetic resonance (NMR) show that, the MICP porosity is 9-10% points lower than HPMI and NMR porosity. Compressibility result shows that deep shale is stiffer in situ than normally assumed in geotechnical modelling and that static compressibility corresponds with dynamic one only at the begining of unloading stress strain data. We found that Kozeny’s modelled permeability fall in the same order of magnitude with measured permeability for shale rich in kaolinite but overestimates permeability by two to three orders of magnitudes for shale with high content of smectite. The empirical Yang and Aplin model gives good permeability estimate comparable to the measured one for shale rich in smectite. This is probably because Yang and Aplin model was calibrated in London clay which is rich in smectite.

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Reservoir Modeling Combining Geostatistics with Markov Chain Monte Carlo Inversion

We present a study on the inversion of seismic reflection data generated from a synthetic reservoir model. Our aim is to invert directly for rock facies and porosity of the target reservoir zone. We solve this inverse problem using a Markov chain Monte Carlo (MCMC) method to handle the nonlinear, multi-step forward model (rock physics and seismology) and to provide realistic estimates of uncertainties. To generate realistic models which represent samples of the prior distribution, and to overcome the high computational demand, we reduce the search space utilizing an algorithm drawn from geostatistics. The geostatistical algorithm learns the multiple-point statistics from prototype models, then generates proposal models which are tested by a Metropolis sampler. The solution of the inverse problem is finally represented by a collection of reservoir models in terms of facies and porosity, which constitute samples of the posterior distribution.

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Organisations: Center for Energy Resources Engineering, National Space Institute, Mathematical and Computational Geoscience
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Sequential hydrogeophysical inversion using airborne EM for 3D hydrostratigraphical zonation

Regional hydrological models are important tools in water resources management. Model prediction uncertainty is primarily due to structural (geological) non-uniqueness which makes sampling of the structural model space necessary to estimate prediction uncertainties. Today geological input to hydrological models is made by geologists, who use cognitive approaches based on geophysical surveys and borehole observations to construct one-truth geological models. Good spatial coverage along with high resolution make airborne time-domain electromagnetic (AEM) data valuable for the hydrostratigraphical input to hydrological models. Geological structures and heterogeneity, which spatially scarce borehole lithology data may overlook, are well resolved in AEM surveys. Due to the discrepancy between hydrological and geophysical parameter spaces the challenge is to translate the electrical resistivity distribution into hydrogeological properties. The translation between hydrological and geophysical parameter space varies spatially and between sites, making a fixed translation insufficient. This study presents a semi-automatic sequential hydrogeophysical inversion method for the integration of AEM and borehole data into regional groundwater models in sedimentary areas, where sand/clay distribution govern groundwater flow. The coupling between hydrological and geophysical parameters is managed using a translator function with spatially variable parameters followed by a 3D zonation. Observed borehole lithologies are represented as clay fractions. The translator function translates the electrical resistivities obtained in a preceding geophysical inversion into clay fractions and is calibrated with observed clay fraction data from boreholes. Principal components are computed for the translated clay fractions and geophysical resistivities. Zonation is carried out by k-means clustering on the principal components. The hydraulic parameters of the zones are determined in a hydrological model calibration using head and discharge observations. The method was applied to field data collected at a Danish field site. The dataset includes interpreted borehole observations and AEM flight path coverage. A classical geological model is available for comparison. Our results show that a competitive hydrological model can be constructed from the AEM dataset using the automatic procedure outlined above. Alternative zonations using various clustering settings, comprising the number of clusters and clustering variables, were evaluated with respect to the performance and prediction uncertainty of the associated hydrological model, and by comparison with the classical geological model.

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Organisations: Department of Environmental Engineering, Water Resources Engineering, Center for Energy Resources Engineering, Department of Applied Mathematics and Computer Science, National Space Institute, Aarhus University
Authors: Marker, P. A. (Intern), Foged, N. (Ekstern), Vest Christiansen, A. (Ekstern), Mosegaard, K. (Intern), Auken, E. (Ekstern), Bauer-Gottwein, P. (Intern)
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Web of Science (2011): Indexed yes
Simulations of Microbial-Enhanced Oil Recovery: Adsorption and Filtration

In the context of microbial-enhanced oil recovery (MEOR) with injection of surfactant-producing bacteria into the reservoir, different types of bacteria attachment and growth scenarios are studied using a 1D simulator. The irreversible bacteria attachment due to filtration similar to the deep bed filtration (DBF) is examined along with the commonly used reversible equilibrium adsorption (REA). The characteristics of the two models are highlighted. The options for bacteria growth are the uniform growth in both phases and growth of attached bacteria only. It is found that uniform growth scenario applied to filtration model provides formation of two oil banks during recovery. This feature is not reproduced by application of REA model or DBF with growth in attached phase. This makes it possible to select a right model based on the qualitative analysis of the experimental data. A criterion is introduced to study the process efficiency: the dimensionless time at which average recovery between pure water injection and maximum surfactant effect is reached. This characteristic recovery period (CRP) was studied as a function of the different MEOR parameters such as bacterial activity, filtration coefficients, and substrate injection concentrations. For both growth scenarios, there is a zone of optimal activity at which the CRP is minimal. Dependence of the CRP on substrate concentration for uniform growth scenario has also an optimal zone. Therefore, growth rate and the substrate concentration should be above a certain threshold value and still not be too high to obtain the minimum CRP. On the other hand, no such zone was found if the bacteria could grow only in the attached phase. Dependencies on both the injected concentration and filtration coefficient are monotonous in this case.
Soft silicone based interpenetrating networks as materials for actuators

A new approach based on silicone interpenetrating networks with orthogonal chemistries has been investigated with focus on developing soft and flexible elastomers with high energy densities and small viscous losses. The interpenetrating networks are made as simple two pot mixtures as for the commercial available silylation based elastomers such as Elastosil RT625. The resulting interpenetrating networks are formulated to be softer than RT625 to increase the actuation caused when applying a voltage due to their softness combined with the significantly higher permittivity than the pure silicone elastomers.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, The Danish Polymer Centre, Center for Energy Resources Engineering
Authors: Yu, L. (Intern), Gonzalez, L. (Intern), Hvilsted, S. (Intern), Skov, A. L. (Intern)
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Title of host publication: Proceedings of SPIE
Volume: 9056
Publisher: SPIE - International Society for Optical Engineering
Article number: 90560C
Main Research Area: Technical/natural sciences
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IPN, Elastomer, Silicone, Dielectric, Thermal stability
DOIs: 10.1117/12.2044769
Source: dtu
Source-ID: u::10829
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Solid formation in piperazine rate-based simulation

Piperazine is a promising solvent for reducing CO2 emissions. It can be applied for the post-combustion capture process and it has limited degradation and fast kinetics. However, precipitation and slurry formation still represent a challenge for the PZ-CO2-H2O system from an operational point of view but also from a modeling perspective. The present work develops a rate-based model for CO2 absorption and desorption modeling for gas-liquid-solid systems and it is demonstrated for the piperazine CO2 capture process. This model is an extension of the DTU CAPCO2 model to
precipitating systems. It uses the extended UNIQUAC thermodynamic model for phase equilibria and thermal properties estimation. The mass and heat transfer phenomena is implemented in a film model approach, based on second order reactions kinetics. The transfer fluxes are calculated using the concentration of the dissolved species since the piperazine is deactivated when present as solid. It is assumed that solid-gas reactions are slow compared to normal liquid side reactions. In the current work, the formation of solids is described in an equilibrium approach, assuming instantaneous formation of hydrates such as PZ·6H2O, PZ·½H2O, and anhydrous PZ. The simulation of a 100t/hr post-combustion capture plant outlines that 5% solid reduces the CO2 capture rate with 13%. Therefore, it demonstrates that an accurate description of the precipitation phenomenon is essential for realistic and accurate modeling.

**General information**

State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering, CERE – Center for Energy Ressources Engineering
Authors: Gaspar, J. (Intern), Thomsen, K. (Intern), von Solms, N. (Intern), Fosbøl, P. L. (Intern)
Pages: 1074-1083
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BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.365 SNIP 0.561 CiteScore 0.92
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.433 SNIP 0.81 CiteScore 1.09
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.425 SNIP 0.785 CiteScore 1.02
ISI indexed (2013): ISI indexed no
Web of Science (2013): Indexed yes
Scopus rating (2012): SJR 0.425 SNIP 0.563 CiteScore 1.08
ISI indexed (2012): ISI indexed no
Web of Science (2012): Indexed yes
Scopus rating (2011): SJR 0.918 SNIP 1.505 CiteScore 2.42
ISI indexed (2011): ISI indexed no
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Web of Science (2009): Indexed yes
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**Strength and Biot’s coefficient for high-porosity oil- or water-saturated chalk**

In the petroleum industry it is relevant to know the Biot coefficient for establishing the effective stresses present in both the overburden and for the reservoir interval. When depleting a reservoir it is important to estimate the settlement through the strain imposed by the effective stress. Also considerations for the size of the drilling window and the magnitude of the
lateral stress involve the Biot coefficient. Additionally, the fluid effect of oil-saturated chalk behaving much stronger than water-saturated chalk affects geomechanical considerations related to e.g. water injection into a reservoir. The Biot coefficient states the degree of cementation or how the pore pressure contributes to the strain resulting from an external load for a porous material. It is here calculated from dynamic measurements and correlated with the strength of outcrop chalk characterized by the onset of pore collapse during hydrostatic loading. The hypothesis is that the Biot coefficient and the theory of poroelasticity may cover the fluid effect by including the increased fluid bulk modulus from oil to water. A high number of test results for both oil- and water-saturated high-porosity outcrop chalk show correlation between the Biot coefficient and the strength.

General information
State: Published
Organisations: Department of Civil Engineering, Section for Geotechnics and Geology, Center for Energy Resources Engineering
Authors: Andreassen, K. A. (Intern)
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Main Research Area: Technical/natural sciences
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author_6937_v4_1.pdf
Source: PublicationPreSubmission
Source-ID: 118925129
Publication: Research - peer-review › Paper – Annual report year: 2015

Synthetic methods in phase equilibria: A new apparatus and error analysis of the method
A new apparatus for the study of high-pressure phase equilibria using a synthetic method is described. The apparatus was especially developed for the study of solubilities of gases in condensed phases, at temperatures ranging from 243 K to 353 K and pressures up to 20 MPa. The quality of the equipment was confirmed through several tests, including measurements along the three phase co-existence line for the system ethane + methanol, the study of the solubility of methane in water, and of carbon dioxide in water. An analysis regarding the application of the synthetic isothermal method in the study of gas solubilities was performed, in order to evaluate the influence of common assumptions and of various experimental aspects on the final solubility results. The analysis revealed that the largest influence on the precision of the solubility results is related to the ratio between the volumes of the two phases in equilibrium. Experiments with small volume of the vapour phase are less susceptible to the influence of other sources of errors, resulting in a higher precision of the final results. © 2013 Elsevier B.V.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering, CERE – Center for Energy Ressources Engineering
Authors: Fonseca, J. (Intern), von Solms, N. (Intern)
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Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 2
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Web of Science (2016): Indexed yes
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Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.139 SNIP 1.461 CiteScore 2.89
The effect of hot water injection on sandstone permeability

Seasonal energy storage can be achieved by hot water injection in geothermal sandstone aquifers. We present an analysis of literature data in combination with new short-term flow through permeability experiments in order to address physical and physico-chemical mechanisms that can alter permeability when sandstones are heated from 20°C to 70–200°C. The pore surface area per unit pore volume was used to normalise permeability data, so that the temperature effect on samples with different pore size could be compared. In sandstones containing the clay mineral kaolinite, heating reduced permeability, suggesting that the observed permeability reduction was due to kaolinite mobilisation. The effect was partly reversible.

General information
State: Published
Organisations: Department of Civil Engineering, Section for Geotechnics and Geology, Center for Energy Resources Engineering, Technical University of Denmark, Geological Survey of Denmark and Greenland
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Pages: 155-166
Publication date: 2014
The Electrical Breakdown of Thin Dielectric Elastomers: Thermal Effects

Dielectric elastomers are being developed for use in actuators, sensors and generators to be used in various applications, such as artificial eye lids, pressure sensors and human motion energy generators. In order to obtain maximum efficiency,
the devices are operated at high electrical fields. This increases the likelihood for electrical breakdown significantly. Hence, for many applications the performance of the dielectric elastomers is limited by this risk of failure, which is triggered by several factors. Amongst others thermal effects may strongly influence the electrical breakdown strength. In this study, we model the electrothermal breakdown in thin PDMS based dielectric elastomers in order to evaluate the thermal mechanisms behind the electrical failures. The objective is to predict the operation range of PDMS based dielectric elastomers with respect to the temperature at given electric field. We performed numerical analysis with a quasi-steady state approximation to predict thermal runaway of dielectric elastomer films. We also studied experimentally the effect of temperature on dielectric properties of different PDMS dielectric elastomers. Different films with different percentages of silica and permittivity enhancing filler were selected for the measurements. From the modeling based on the fitting of experimental data, it is found that the electrothermal breakdown of the materials is strongly influenced by the increase in both dielectric permittivity and conductivity.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, The Danish Polymer Centre, Center for Process Engineering and Technology, Center for Energy Resources Engineering, Delft University of Technology, Danfoss PolyPower A/S
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Publisher: SPIE - International Society for Optical Engineering
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Conference: SPIE Smart Structures/NDE, San Diego, CA, United States, 09/03/2014 - 09/03/2014
DEAP, PDMS, Electrothermal breakdown, Numerical method
Electronic versions:
prod11392294947007.The_Electrical_Breakdown_of_Thin_Dielectric_Elastomers_Thermal_Effects.pdf
DOIs:
10.1117/12.2037292
Publication: Research - peer-review › Article in proceedings – Annual report year: 2014

Thermodynamic modeling of complex systems
Offshore reservoirs represent one of the major growth areas of the oil and gas industry, and environmental safety is one of the biggest challenges for the offshore exploration and production. The oil accidents in the Gulf of Mexico in 1979 and 2010 were two of the biggest disasters in history. Contrary to earlier theories, the oil is not only present on the surface, but also in great volumes both in the water column and on the seafloor, which indicates that we do not know enough about how oil behaves in water and interacts with it. Sonar detection is one of the most important and necessary technologies to reduce the environmental effects of offshore oil exploration. It could be used (1) to detect oil and gas leaks around the subsea well head enabling faster responses, especially in deep water and/ or ice covered areas; (2) to detect and map the oil in the seawater column during cleanup process after an oil spill. Engineering thermodynamics could be applied in the state-of-the-art sonar products through advanced artificial technology, if the speed of sound, solubility and density of oil-seawater systems could be satisfactorily modelled. The addition of methanol or glycols into unprocessed well streams during subsea pipelines is necessary to inhibit gas hydrate formation, and the offshore reservoirs often mean complicated temperature and pressure conditions. Accurate description of the phase behavior and thermophysical properties of complex systems containing petroleum fluids and polar compounds are extremely important from viewpoints of the economical operation and environmental safety. The classical thermodynamic models used by the oil industry are semi-empirical and not suitable for mixtures containing water and other polar chemicals. The complex nature of water, its anomalous properties due to hydrogen bonding and the hydrophobic interactions with hydrocarbons (oils), are not described well by such simple models. The perturbation theory based models have an explicit term to account for the hydrogen bonding, and these models are also believed to have better performance for derivative properties, e.g. speed of sound, and for density under extreme conditions. This PhD thesis studies the capabilities and limitations of the Perturbed-Chain Statistical Association Fluid Theory (PC-SAFT) equation of state. It consists of three parts. In the first part, the PC-SAFT EOS is successfully applied to model the phase behaviour of water, chemical and hydrocarbon (oil) containing systems with newly developed pure component parameters for water and chemicals and characterization procedures for petroleum fluids. The performance of the PC-SAFT EOS on liquid-liquid equilibria of water with hydrocarbons has been under debate for some v7 years. An interactive step-wise procedure is proposed to fit the model parameters for small associating fluids by taking the liquid-liquid equilibrium data into account. It is still far away from a simple task to apply PC-SAFT in routine PVT simulations and phase behaviour of petroleum fluids. It has been extensively studied on how to develop general petroleum fluid characterization approaches for PC-SAFT. The performance of the newly developed parameters and characterization procedures for the description of the phase equilibria of well- and ill-defined binary and ternary systems containing water, chemicals and/or hydrocarbons (oils) is quite satisfactory, if compared to the models available in literature. The modeling of petroleum fluid-water-MEG systems provides further information to develop simpler
and more robust characterization approaches. In the second part, the speed of sound data and their correlations of various systems are reviewed. Two approaches are proposed to improve the speed of sound description within the PC-SAFT framework by putting speed of sound data into the parameter estimation and/or the universal constant regression. The first approach works only for short associating fluids, while the second approach significantly improves the speed of sound description for various systems both qualitatively and quantitatively. The possibility of simultaneous modeling of phase behavior and speed of sound, including the effects of parameter estimation approaches for 1-alcohol containing systems, are also investigated. In the third part, the fundamentals of PC-SAFT are investigated based on the universal constant regression. The PC-SAFT EOS has been criticized for some numerical pitfalls during the recent years. A new variant of universal constants has been developed, which has avoided the numerical pitfalls of having more than three volume roots in the real application range. It has been shown that it is possible to directly use the original PC-SAFT parameters with the new universal constants for the systems considered in this thesis. Finally, the salt effects on the solubility of hydrocarbons, the speed of sound, and the static permittivity of aqueous solutions are briefly discussed. It is still an open question how to estimate the model parameters for associating fluids with pure component properties only. The possibility of using the static permittivity data in the parameter estimation is discussed by adopting a newly developed theory of static permittivity and association theory based EOS.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering, Department of Chemistry
Authors: Liang, X. (Intern), Kontogeorgis, G. (Intern), Thomsen, K. (Intern), Yan, W. (Intern)
Number of pages: 287
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Source: PublicationPreSubmission
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Publication: Research › Ph.D. thesis – Annual report year: 2015

The role of monomer fraction data in association theories—Can we improve the performance for phase equilibrium calculations?
Monomer fraction (fraction of non-hydrogen bonded molecules) data obtained from spectroscopy are available for a few associating compounds. Such data can be used for testing the performance of association models like CPA and SAFT or alternatively be employed in the model development. But how accurate and how useful are such data today and how successful is their use in the context of association models? In this work we attempt to answer these questions in the case of the CPA model and for ethanol. CPA has been already successfully used to describe thermodynamic properties of many ethanol containing mixtures, using an ethanol parameter set that was adjusted to experimental vapor pressure and liquid density data. We present in this work a new parameter set for ethanol which is estimated using experimental vapor pressure, liquid density data as well as the experimental monomer fractions for liquid ethanol. Using both the existing (“old”) and the new parameter sets, we perform an extensive comparison of CPA results for a wide range of ethanol-containing systems, with water and alkanes as well as multicomponent water–ethanol–hydrocarbon liquid–liquid equilibria and hydrate curves with different ethanol content as inhibitor. There are some differences in the performance of CPA with the two sets but on average the results are similar. This may indicate that monomer fraction data are not very useful in this case or that ethanol monomer fraction data are not accurate and both possibilities are discussed.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering, CHEC Research Centre, Center for Energy Resources Engineering
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The Virtual Product-Process Design Lab

General information
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Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Center for Energy Resources Engineering, CERE – Center for Energy Ressources Engineering
Authors: Kalakul, S. (Intern), Kontogeorgis, G. (Intern), Gani, R. (Intern)
Publication date: 2014
Event: Abstract from 2014 AIChE Annual Meeting: American Institute of Chemical Engineers, Atlanta, United States.
Main Research Area: Technical/natural sciences
Electronic versions:
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Source: PublicationPreSubmission
Source-ID: 103645344
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The Virtual Product-Process Design Laboratory for Structured Chemical Product Design and Analysis
The objective of this paper is to present new methods for design of chemicals based formulated products and their implementation in the software, the Virtual Product-Process Design Laboratory. The new products are tailor-made blended liquid products and emulsion-based products. The new software employs a template approach, where each template follows the same common steps in the workflow for design of formulated products, but has the option to employ different product specific property models, data and calculation routines, when necessary. With the new additions, the software is able to support the design and analysis of a wide range of homogeneous formulated products: tailor-made blends, single phase liquid formulations and emulsion-based products. The decision making process is supported by dedicated property models and structured databases, specifically developed for each design problem scenario. Output from the software is a small set of most promising product candidates and a short list of recommended experiments that can validate and further fine-tune the product composition. The application of the new features is highlighted through two case studies relative to an emulsion-based product and a tailor-made blend

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Center for Energy Resources Engineering, CERE – Center for Energy Ressources Engineering
Authors: Mattei, M. (Intern), Yunus, N. A. B. (Intern), Kalakul, S. (Intern), Kontogeorgis, G. (Intern), Woodley, J. (Intern), Gernaey, K. (Intern), Gani, R. (Intern)
Pages: 61-66
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UV-Cured, Platinum-Free, Soft Poly(dimethylsiloxane) Networks
To overcome the drawbacks exhibited by platinum-catalyzed curing of silicones, photoinitiated thiol–ene cross-linking of high-molecular-weight poly(dimethylsiloxane) (PDMS) prepolymer has been investigated as a pathway to novel soft PDMS networks, based on commercially available starting materials was developed. Through a fast and efficient two-step cross-linking reaction highly flexible PDMS elastomers were prepared.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, The Danish Polymer Centre, Center for Energy Resources Engineering
Authors: Goswami, K. (Intern), Skov, A. L. (Intern), Daugaard, A. E. (Intern)
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Main Research Area: Technical/natural sciences

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Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 5.03 SJR 2.247 SNIP 1.046
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 2.416 SNIP 1.184 CiteScore 4.99
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 2.487 SNIP 1.219 CiteScore 5.51
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 2.604 SNIP 1.239 CiteScore 5.68
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 2.884 SNIP 1.294 CiteScore 5.55
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 2.726 SNIP 1.336 CiteScore 5.46
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 2.527 SNIP 1.292
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 2.499 SNIP 1.365
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 2.887 SNIP 1.407
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 3.233 SNIP 1.532
Scopus rating (2006): SJR 2.911 SNIP 1.505
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 2.62 SNIP 1.454
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 2.32 SNIP 1.472
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 2.156 SNIP 1.45
Web of Science (2003): Indexed yes
Vapor-Liquid Equilibrium of Methane with Water and Methanol. Measurements and Modeling

There is a need for high-quality experimental phase equilibrium data in the petroleum and chemical industries, for example, mixtures of oil and gas with gas hydrate inhibitors (methanol, glycols) and organic acids. This includes a wide range of different systems, which all deal with processes that rely on phase equilibrium data for optimization. The objective of this work is to provide experimental data for hydrocarbon systems with polar chemicals such as alcohols, glycols, and water. New vapor-liquid equilibrium data are reported for methane + water, methane + methanol, and methane + methanol + water for several temperatures in the range 284 K to 324 K and in the pressure range (5 to 20) MPa. The Cubic-Plus-Association (CPA) equation of state is used to model the phase equilibria data measured. A good agreement between predictions and experimental data is observed, supporting the reliability of the new data.

General information
State: Published
Organisations: Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering
Authors: Frost, M. G. (Intern), Karakatsani, E. (Intern), von Solms, N. (Intern), Richon, D. (Intern), Kontogeorgis, G. (Intern)
Pages: 961-967
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Main Research Area: Technical/natural sciences

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Volume: 59
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BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.29 SJR 0.88 SNIP 1.097
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.868 SNIP 0.966 CiteScore 1.96
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.021 SNIP 1.208 CiteScore 2.22
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.135 SNIP 1.199 CiteScore 2.17
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.141 SNIP 1.103 CiteScore 2.01
ISI indexed (2012): ISI indexed yes
The existence of short-chain domains in heterogeneous bimodal PDMS networks has been confirmed visually, for the first time, through confocal fluorescence microscopy. The networks were prepared using a controlled reaction scheme where short PDMS chains were reacted below the gelation point into hyperbranched structures using a fluorescent silicone compatible cross-linker. The formation of the hyperbranched structures was confirmed by FTIR, 1H-NMR and size exclusion chromatography (SEC). The short-chain hyperbranched structures were thereafter mixed with long-chain hyperbranched structures to form bimodal networks with short-chain domains within a long-chain network. The average sizes of the short-chain domains were found to vary from 2.1 to 5.7 mm depending on the short-chain content. The visualised network structure could be correlated thereafter to the elastic properties, which were determined by rheology. All heterogeneous bimodal networks displayed significantly lower moduli than mono-modal PDMS elastomers prepared from the long polymer chains. Low-loss moduli as well as low-sol fractions indicate that low-elastic moduli can be obtained without compromising the network's structure.
Acid Gas Removal from Natural Gas with Alkanolamines: A Modeling and Experimental Study

Some 40% of the world’s remaining gas reserves are sour or acid, containing large quantities of CO₂ and H₂S and other sulfur compounds. Many large oil and gas fields have more than 10 mole % CO₂ and H₂S content. In the gas processing industry absorption with chemical solvents has been used commercially for the removal of acid gas impurities from natural gas. Alkanolamines, simple combinations of alcohols and ammonia, are the most commonly used category of chemical solvents for acid gas capture. This Ph.D. project is about thermodynamics of natural gas cleaning process with alkanolamines as solvent, modeling and experimental study. The project is collaboration between DTU and Statoil. Thermodynamic modeling is being done at DTU and experiments were performed at Statoil laboratories. In modeling part of the project, thermodynamic models were developed for CO₂-MDEA-H₂O, CO₂-MEA-H₂O, CO₂-MDEA-MEA-H₂O, H₂S-MDEA-H₂O, H₂S-MCH₄-MDEA-H₂O systems and the constituent binary subsystems of the mentioned mixtures. The experimental part of the project includes vapor-liquid equilibrium measurements for CO₂-MDEA-H₂O and CO₂-MDEA-PZ-H₂O at atmospheric pressure, high pressure vapor-liquid equilibrium experiments for H₂S-MCH₄-MDEA-H₂O, density measurements for aqueous MDEA and aqueous activated MDEA and piperazine solubility measurements in aqueous MDEA. Different commercial simulators together with the developed Extended UNIQUAC model were used to simulate the experimental data points. The effect of total pressure on acid gas solubility was also quantitatively investigated through both experimental and modeling approaches.

General information
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A Comparative Study of Reduced-Variables-Based Flash and Conventional Flash
For compositional transient simulations including compositional reservoir simulations, phase-equilibrium calculation, often formulated as a flash problem, can be time consuming. It is therefore important to speed up the calculation of phase equilibrium to improve the efficiency of the simulator. The reduced-variables methods, or the reduction methods, reformulate the original phase equilibrium problem with a smaller set of independent variables. Various versions of the reduced-variables methods have been proposed since the mid-1980s. The methods were first proposed for cubic equations of state (EOSs) with zero binary-interaction parameters (BIPs) and later generalized to situations with nonzero-BIP matrices. Most of the studies in the last decade suggest that the reduced-variables methods are much more efficient than the conventional flash method. However, Haugen and Beckner (2011) questioned the advantages of the reduced-variables methods in their recent paper. A fair comparison between the reduced-variables-based flash and the conventional flash is not straightforward because it is difficult to formulate the former as unconstrained minimization problems, and the flash calculation time is also related to the implementation quality. With the recent formulations by Nichita and Gracia (2011), it is possible to code the reduced-variables methods without extensive modifications of Michelsen’s conventional flash algorithm. A minimization-based reduced-variables algorithm was coded and compared with the conventional minimization-based flash. A test with the use of the SPE 3 example (Kenyon and Behie 1987) showed that the best reduction in time was less than 20% for the extreme situation of 25 components and just one row/column with nonzero BIPs. A better performance can be achieved by a simpler implementation directly using the sparsity of the BIP matrix.

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Organisations: Department of Chemistry, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering, Center for Energy Resources Engineering, Technical University of Denmark
Authors: Yan, W. (Intern), Stenby, E. H. (Intern), Michelsen, M. L. (Intern)
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A Dantzig-Wolfe Decomposition Algorithm for Economic MPC of Distributed Energy Systems

In economic model predictive control of distributed energy systems, the constrained optimal control problem can be expressed as a linear program with a block-angular structure. In this paper, we present an efficient Dantzig-Wolfe decomposition algorithm specifically tailored to problems of this type. Simulations show that a MATLAB implementation of the algorithm is significantly faster than several state-of-the-art linear programming solvers and that it scales in a favorable way.

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Organisations: Department of Applied Mathematics and Computer Science, Scientific Computing, Center for Energy Resources Engineering, DONG Energy A/S
Authors: Sokoler, L. E. (Intern), Standardi, L. (Intern), Edlund, K. (Ekstern), Jørgensen, J. B. (Intern)
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A Fast Condensing Method for Solution of Linear-Quadratic Control Problems

In both Active-Set (AS) and Interior-Point (IP) algorithms for Model Predictive Control (MPC), sub-problems in the form of linear-quadratic (LQ) control problems need to be solved at each iteration. The solution of these sub-problems is usually the main computational effort. In this paper we consider a condensing (or state elimination) method to solve an extended version of the LQ control problem, and we show how to exploit the structure of this problem to both factorize the dense Hessian matrix and solve the system. Furthermore, we present two efficient implementations. The first implementation is formally identical to the Riccati recursion based solver and has a computational complexity that is linear in the control horizon length and cubic in the number of states. The second implementation has a computational complexity that is quadratic in the control horizon length as well as the number of states. When the state dimension is high, this implementation is faster than the Riccati recursion based implementation.

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Authors: Frison, G. (Intern), Jørgensen, J. B. (Intern)
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A Grey-Box Model for Spray Drying Plants

Multi-stage spray drying is an important and widely used unit operation in the production of food powders. In this paper we develop and present a dynamic model of the complete drying process in a multi-stage spray dryer. The dryer is divided into three stages: The spray stage and two fluid bed stages. Each stage is assumed ideally mixed and described by mass- and energy balances. The model is able to predict the temperature, the residual moisture and the particle size in each stage. Process constraints are also proposed to predict deposits due to stickiness of the powder. The model predictions are compared to datasets gathered at GEA Process Engineering’s test facility. The identified grey-box model parameters are identified from data and the resulting model fits the data well. The complexity of the model has been selected such that it is suitable for development of real-time optimization algorithms in an economic optimizing MPC framework.
Alternative Layouts for the Carbon Capture with the Chilled Ammonia Process

Many alternatives are being investigated for the carbon capture, but none appears to have been proved as the choice for full-scale applications. This work considers the Chilled Ammonia Process for coal-fired Ultra Super Critical power plants. Three layouts are simulated with Aspen Plus and the Extended UNIQUAC thermodynamic model. Compared to a traditional layout, stripping of the wash water of the absorber or, better, splitting the rich solution between the middle and the top of the column limits greatly the ammonia slip. Moreover, splitting the regeneration over two levels reduces substantially the electric loss due to stream extraction from the turbine. The simulations show that the net electric efficiency drops from 45.5% to 33.5-34.5%, the SPECCA index is 3.8-4.3 MJth kgCO2–1 and the heat duties are 2.7-2.9 MJth kgCO2–1. The performances may improve greatly upon optimization of the parameters.
A new pilot absorber for CO2 capture from flue gases: Measuring and modelling capture with MEA solution

A pilot absorber column for CO2 recovery from flue gases was constructed and tested with aqueous 30wt% monoethanolamine (MEA), a primary amine, as capture solvent. The pilot plant data were compared with a mathematical rate based packed-column model. The simulation results compared well with the pilot plant data. The packed height of the column can be varied from 1.6 to 8.2 m by means of five different liquid inlets. The column has an inner diameter of 100 mm and is packed with structured Mellapak 250Y packing. Counter-current flow is used. The pilot plant performance was investigated by changing three parameters: the absorption height, liquid flow rate, and the loading of lean MEA. This was done using a synthetic flue gas consisting of 10% CO2 with a flow rate of approximately 33 m³/h at ambient temperature and atmospheric pressure. 23 runs were performed. It was observed that while CO2 recovery increases with an increase in flow rate of absorbent and absorption height, it decreases as the lean CO2-loading of the absorbent increases. In addition it has been possible to obtain temperature bulges in the bottom part of the absorber by the applied operation conditions. Bulges are observed at liquid flows around 4.2 L/min and below. The results showed that is was possible to achieve 80% recovery with 3.3 m absorption height and a liquid flow of 2.1L/min. The simulations show good agreement with the experimental values, although slight deviations arise as the CO2-loading increases and the temperature bulge becomes more distinct.

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Organisations: Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Ressources Engineering, CHEC Research Centre
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An Implementation of the Frequency Matching Method

During the last decade multiple-point statistics has become increasingly popular as a tool for incorporating complex prior information when solving inverse problems in geosciences. A variety of methods have been proposed but often the implementation of these is not straightforward. One of these methods is the recently proposed Frequency Matching method to compute the maximum a posteriori model of an inverse problem where multiple-point statistics, learned from a training image, is used to formulate a closed form expression for an a priori probability density function. This paper discusses aspects of the implementation of the Frequency Matching method and the techniques adopted to make it computationally feasible also for large-scale inverse problems. The source code is publicly available at GitHub and this paper also provides an example of how to apply the Frequency Matching method to a linear inverse problem.

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Application of the cubic-plus-association (CPA) equation of state to model the fluid phase behaviour of binary mixtures of water and tetrahydrofuran

The complex fluid phase behaviour of the binary system comprised of water and tetrahydrofuran (THF) is modelled by use of the cubic-plus-association (CPA) equation of state. A total of seven modelling scenarios are analysed, differing only in their way of describing THF and its interactions (hydrogen bonding) with water. The qualitative behaviour of the fluid phase equilibria in this system can only be described by CPA when cross-association between water and THF is allowed. Six of the seven tested modelling scenarios allow for cross-association between the two compounds. These scenarios are named Case 2 to Case 7. Case 2 treats THF as non self-associating, but applies a single association site on the THF oxygen atom, that allows for cross-linking with a single water molecule. Case 3 is identical to Case 2 but applies two association sites on THF, allowing for simultaneous cross-association with two water molecules. Case 4 treats THF as self-associating and cross-associating according to an association scheme with two electron accepting sites and a single electron donating site. Case 5 also considers both self- and cross-association by THF, but applies an association scheme with two electron accepting- and two electron donating sites. Cases 6 and 7 are similar to Cases 4 and 5, respectively, however the binary cross-association volume between electron accepting sites on water and electron donating sites on THF is adjusted to match the CPA descriptions with available experimental VLE data. It is found that Cases 2, 3, 6 and 7 (when applying three adjustable binary parameters), are the only cases, which can describe both VLE and LLE using a single set of parameters. With a total of three binary parameters correlated to available VLE data, these data may be described with average absolute deviations of approximately 5–7 percent. The LLE is well predicted by both model Cases 2 and 3, with a slightly better phase composition prediction by Case 3. While Cases 6 and 7 describe VLE data better than the cases treating THF as solvating, the LLE is less accurately described. Based on the results presented in this work, it is suggested to model this binary system considering THF as cross-associating only, with two cross-association sites. The use of a temperature dependent binary interaction parameter and a correlated binary cross-association volume then allows for both accurate VLE and LLE descriptions in large ranges of temperature and pressure.

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A Riccati Based Homogeneous and Self-Dual Interior-Point Method for Linear Economic Model Predictive Control

In this paper, we develop an efficient interior-point method (IPM) for the linear programs arising in economic model predictive control of linear systems. The novelty of our algorithm is that it combines a homogeneous and self-dual model, and a specialized Riccati iteration procedure. We test the algorithm in a conceptual study of power systems management. Simulations show that in comparison to state of the art software implementation of IPMs, our method is significantly faster and scales in a favourable way.

**General information**

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**Organisations:** Department of Applied Mathematics and Computer Science, Scientific Computing, Center for Energy Resources Engineering, DONG Energy A/S

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Authors: Fournier, A. (Ekstern), Mosegaard, K. (Intern), Omre, H. (Ekstern), Sambridge, M. (Ekstern), Tenorio, L. (Ekstern)
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Scopus rating (2014): SJR 1.413 SNIP 1.434 CiteScore 1.9
Web of Science (2014): Indexed yes
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Scopus rating (2012): SJR 1.693 SNIP 1.837 CiteScore 2.04
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Thermodynamics plays an important role in many applications in the petroleum industry, both upstream and downstream, ranging from flow assurance, (enhanced) oil recovery and control of chemicals to meet production and environmental regulations. There are many different applications in the oil & gas industry, thus thermodynamic data (phase behaviour, densities, speed of sound, etc) are needed to study a very diverse range of compounds in addition to the petroleum ones (CO2, H2S, water, alcohols, glycols, mercaptans, mercury, asphaltene, waxes, polymers, electrolytes, biofuels, etc) within a very extensive range of conditions, up to very high pressures. Actually, the petroleum industry was one of the first industrial sectors which used extensively thermodynamic models and even contributed to the development of several of the most popular and still widely used approaches. While traditional thermodynamic models like cubic equations of state have been the dominating tools in the petroleum industry, the focus of this review is on the association models. Association models are defined as the models of SAFT/CPA family (and others) which incorporate hydrogen bonding and other complex interactions. Such association models have been, especially over the last 20 years, proved to be very successful in predicting many thermodynamic properties in the oil & gas industry. They have not so far replaced cubic equations of state, but the results obtained by using these models are very impressive in many cases, e.g., for gas hydrate related systems, CO2/H2S mixtures, water/hydrocarbons and others. This review highlights both the major advantages of these association models and some of their limitations, which we believe should be discussed in the future.
Association theories for complex thermodynamics

Thermodynamics of complex systems (e.g. with associating molecules, multicomponent mixtures, multiphase equilibria, wide ranges of conditions, estimation of many different properties simultaneously) is a topic of great importance in chemical engineering and for a wide range of industrial applications. While specialized models can handle different cases, even complex ones, with the advent of powerful theories and computers there is the hope that a single or a few models could be suitable for a general modeling of complex thermodynamics. After more than 100 years with active use of thermodynamic models, we have now come to the understanding that simple one-fluid theories like the cubic equations of state or the various forms of local composition models will never be able to model a wide range of complex systems with sufficient accuracy. While various modern approaches have appeared, one very promising direction for a general and useful for engineering purposes modeling of complex thermodynamics is via the use of association theories e.g. those based on chemical theory (like APACT), or on the lattice theory (like NRHB) or those based on perturbation theory (like SAFT and CPA). The purpose of this review is two-fold: first to illustrate some of the significant capabilities of these association theories and why indeed they have already been extensively used and are expected to find even more applications in the future. The second and most important aspect of this review is to outline many of the non-answered questions about these association theories, provide answers to some of these questions and limitations based on recent research and highlight areas where further research is needed.
A Theoretical Analysis of Colloid Attachment and Straining in Chemically Heterogeneous Porous Media

A balance of applied hydrodynamic (TH) and resisting adhesive (TA) torques was conducted over a chemically heterogeneous porous medium that contained random roughness of height $h_r$ to determine the fraction of the solid surface area that contributes to colloid immobilization ($S_f^*$) under unfavorable attachment conditions. This model considers resistance due to deformation and the horizontal component of the adhesive force ($F_A$), spatial variations in the pore scale velocity distribution, and the influence of $h_r$ on lever arms for TH and TA. Values of $S_f^*$ were calculated for a wide range of physicochemical properties to gain insight into mechanisms and factors influencing colloid immobilization. Colloid attachment processes were demonstrated to depend on solution ionic strength (IS), the colloid radius ($r_c$), the Young’s modulus ($K$), the amount of chemical heterogeneity ($P^+$), and the Darcy velocity ($q$). Colloid immobilization was also demonstrated to occur on a rough surface in the absence of attachment. In this case, $S_f^*$ depended on IS, $r_c$, the roughness fraction ($f$), $h_r$, and $q$. Roughness tended to enhance TA and diminish TH. Consequently, the effect of IS on $S_f^*$ was enhanced by $h_r$ relative to attachment. In contrast, the effects of $r_c$ and $q$ on $S_f^*$ were diminished by $h_r$ in comparison to attachment. Colloid immobilization adjacent to macroscopic roughness locations shares many similarities to grain–grain contact points and may be viewed as a type of straining process. In general, attachment was more important for higher IS and variance in the secondary minimum, and for smaller $r_c$, $q$, and $K$, but diffusion decreased these values. Conversely, straining was dominant for the opposite conditions. Discrepancies in the literature on mechanisms of colloid retention are likely due to a lack of consideration of all of these factors.
A Tuning Procedure for ARX-based MPC

We present an optimization based tuning procedure with certain robustness properties for an offset free Model Predictive Controller (MPC). The MPC is designed for univariate processes that can be represented by an ARX model. The advantage of ARX model representations is that standard system identification techniques using convex optimization can be used for identification of such models from input-output data. The stochastic model of the ARX model identified from input-output data is modified with an ARMA model designed as part of the MPC-design procedure to ensure offset-free control. The ARMAX model description resulting from the extension can be realized as a state space model in innovation form. The MPC is designed and implemented based on this state space model in innovation form. Expressions for the closed-loop dynamics of the unconstrained system is used to derive the sensitivity function of this system. The closed-loop expressions are also used to numerically evaluate absolute integral performance measures. Due to the closed-loop expressions, these evaluations can be done relatively quickly. Consequently, the tuning may be performed by numerical minimization of the integrated absolute error subject to a constraint on the maximum of the sensitivity function. The latter constraint provides a robustness measure that is essential for the procedure.

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A Tuning Procedure for ARX-based MPC of Multivariate Processes

We present an optimization based tuning procedure with certain robustness properties for an offset free Model Predictive Controller (MPC). The MPC is designed for multivariate processes that can be represented by an ARX model. The stochastic model of the ARX model identified from input-output data is modified with an ARMA model designed as part of the MPC-design procedure to ensure offset-free control. The ARMAX model description resulting from the extension can be realized as a state space model in innovation form. Expressions for the closed-loop dynamics of the unconstrained system is used to derive the sensitivity function of this system. The closed-loop expressions are also used to numerically evaluate absolute integral performance measures. Due to the closed-loop expressions these evaluations can be done relative quickly. Consequently, the tuning may be performed by numerical minimization of the integrated absolute error subject to a constraint on the maximum of the sensitivity function. The latter constraint provides a robustness measure that is essential for the procedure. The method is demonstrated for two simulated examples: A Wood-Berry distillation column example and a cement mill example.

General information
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A Warm-Started Homogeneous and Self-Dual Interior-Point Method for Linear Economic Model Predictive Control

In this paper, we present a warm-started homogenous and self-dual interior-point method (IPM) for the linear programs arising in economic model predictive control (MPC) of linear systems. To exploit the structure in the optimization problems, our algorithm utilizes a Riccati iteration procedure which is adapted to the non-standard system solved in homogenous and self-dual IPMs, and specifically tailored to economic MPC. Fast convergence is further achieved by means of a recent warm-starting strategy for homogenous and self-dual IPMs that has not previously been applied to MPC. We implement our algorithm in MATLAB and its performance is analyzed based on a smart grid power management case study. Closed loop simulations show that 1) our algorithm is significantly faster than state-of-the-art IPMs based on sparse linear algebra routines, and 2) warm-starting reduces the number of iterations by approximately 15-35%.

Binary and ternary VLE of the 2-(diethylamino)-ethanol (DEEA)/ 3-(methylamino)-propylamine (MAPA)/ water system

A mixed 2-(diethylamino)-ethanol (DEEA) and 3-(methylamino)-propylamine (MAPA) system could be an attractive alternative solvent to improve the performance of CO2 capture for low partial pressure cases. This solvent has the advantages of forming two liquid phases upon CO2 loading, one rich in CO2 and the other very low in CO2. Having a highly concentrated rich solvent improvements could be reached by reducing the sensible heat and improving the equilibrium sensitivity hence reducing the need for stripping steam. Also it is possible that the heat of absorption may change to the better. To better understand this system in designing the separation unit requires substantial work on characterization of the solvent. One important aspect is to provide equilibrium data. In this work new ebulliometric VLE data for the binary DEEA/H2O and DEEA/MAPA systems and the ternary DEEA/MAPA/H2O system are reported at different temperatures and concentrations. Results show that pure MAPA is more volatile than DEEA, but in aqueous solution MAPA was found to be less volatile. A mix of DEEA and MAPA in aqueous solution tends to lower the volatility thus makes the system more advantageous by reducing volatility. The activity coefficients for the species in the ternary aqueous system are found to be lower than the activity coefficients obtained from the corresponding binary aqueous
mixtures. The UNIQUAC framework was implemented to represent the experimental data. The six UNIQUAC parameters were determined and were able to predict P-T-x-y, activity coefficient, excess enthalpy and freezing point depression for both the binary and ternary systems. However, a small inconsistency was observed between water activity coefficients determined from ebulliometer and freezing point depression measurements.

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ISI indexed (2011): ISI indexed yes
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BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.319 SNIP 1.708
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Web of Science (2007): Indexed yes
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BINARY VLE of DEEA/H2O, MAPA/H2O and DEEA/MAPA SYSTEMS

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Activities:

Burial diagenesis of deep sea chalk as reflected in Biot's coefficient
Burial diagenesis of chalk has been widely studied, but little agreement has been reached on by which mechanism porosity declines, and on how to calculate the deforming stress in the most informative way. Data from Ocean Drilling Program show that calcareous ooze transforms to chalk and chalk to limestone as burial increases and porosity decreases. The porosity decrease is accompanied by an increasing velocity to elastic waves, and consequently a decreasing Biot's coefficient, as estimated from velocity and density of core samples. When the effective burial stress is normalized to total horizontal cross sectional area, the porosity is found to decline as a function of stress. The porosity trend proceeds smoothly from ooze over chalk to limestone. By contrast, when vertical effective stress is normalized to grain contact area, each lithology shows a distinct porosity-decline - stress pattern. In the ooze, we find that the natural compaction causes an increasing stress on grain contact area, indicating that the ooze particles become strongly strained. In the chalk section, contact cement is probably the reason why particles become less strained as porosity declines. In the limestone, stress on particles apparently is low and not correlated with porosity, probably because the pore-filling cementation in this interval causes Biot's coefficient to decline as burial increases. Limestone from the water zone of the North sea Chalk Group follows the same stress trend as deep sea limestone. These results indicate that by normalizing effective stress to grain contact area, we can get information about the mechanism behind burial related diagenetic porosity decline.

General information
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Burial diagenesis of deep sea chalk as reflected in Biot's coefficient

Burial diagenesis of chalk has been widely studied, but little agreement has been reached on by which mechanism porosity declines, and on how to calculate the deforming stress in the most informative way. Data from Ocean Drilling Program show that calcareous ooze transforms to chalk and chalk to limestone as burial increases and porosity decreases. The porosity decrease is accompanied by an increasing velocity to elastic waves, and consequently a decreasing Biot's coefficient, as estimated from velocity and density of core samples. When the effective burial stress is normalized to total horizontal cross sectional area, the porosity is found to decline as a function of stress. The porosity trend proceeds smoothly from ooze over chalk to limestone. By contrast, when vertical effective stress is normalized to grain contact area, each lithology shows a distinct porosity-decline - stress pattern. In the ooze, we find that the natural compaction causes an increasing stress on grain contact area, indicating that the ooze particles become strongly strained. In the chalk section, contact cement is probably the reason why particles become less strained as porosity declines. In the limestone, stress on particles apparently is low and not correlated with porosity, probably because the pore-filling cementation in this interval causes Biot's coefficient to decline as burial increases. Limestone from the water zone of the North sea Chalk Group follows the same stress trend as deep sea limestone. These results indicate that by normalizing effective stress to grain contact area, we can get information about the mechanism behind burial related diagenetic porosity decline.

Capabilities and limitations of predictive engineering theories for multicomponent adsorption

Multicomponent adsorption of gas mixtures on diverse solid surfaces is important in many applications. However, there are still many questions on the practical applicability of the available theories, especially for polar systems. In this work, we consider three well-known theories suitable for the prediction of multicomponent adsorption with parameters obtained solely from correlating single gas/solid data. We have tested them over an extensive database with emphasis on polar systems (both gases and solids). The three theories are the multicomponent Langmuir, the ideal adsorbed solution theory (IAST), and the multicomponent potential adsorption theory (MPTA). We have not attempted to improve/modify the methods in any way but have used them in their original form, as the purpose of our work is to illustrate the capabilities and inherent limitations of the models for predicting multicomponent adsorption. We have ensured that the description of single gas/solid systems is as accurate as possible, but besides this, the calculations for multicomponent systems are straight predictions. The work revealed on one side that all three theories yield for some systems similar predictions, with IAST and MPTA performing overall better than the multicomponent Langmuir. On the other hand, it is also shown that all the three theories, despite the good results in some cases, have serious limitations particularly for water and to some extent also for certain polar solids. Both strengths and weaknesses of the three models are discussed. © 2013 American Chemical Society.
Biot's effective stress coefficient ($\alpha$) is a measure of how well grains in the rocks are connected with each other. The amount of contact cements between the grains determines the stiffness of rocks. Change in grain contact occurs during natural diagenesis of sedimentary rock. Contact between the grains could also change during elastic deformation of the grains in a rock mechanics test. Diagenetic change in grain contact cement of chalk can be compared with stress-induced change in the laboratory. The change in porosity is studied with reference to the change in effective stress on grain contacts ($\sigma_m^\prime$). The porosity reduction trend with change in $\alpha_m$ indicates that in newly deposited calcareous sediment (in Kerguelen Plateau), porosity reduces at a faster rate, as $\alpha_m$ decreases until $\alpha$ decreased below 0.95. As contact area between the grains increases (decrease in $\alpha$), $\sigma_m^\prime$ decreases and porosity reduces at a slower rate. We noticed that presence of non carbonates and hydrocarbon could increase $\sigma_m^\prime$. During rock mechanics test in the lab, with increased applied stress, $\sigma_m^\prime$ increases, Biot's effective stress coefficient shows a decreasing trend, while a minor porosity reduction was observed. © 2013 American Society of Civil Engineers.
Composition of in situ burn residue as a function of weathering conditions
Troll B crude oil was weathered under Arctic conditions with different ice coverage: open water, 50% ice and 90% ice. Samples (100 mL) were taken during the experiment and tested for ignitability in a burning cell. From each burning a residue sample was taken for analysis. The burning process removed the light compounds eluting before C13. No effect from the prior weathering time or the different ice coverage was seen in the burn residue composition. The content of selected Poly Aromatic Hydrocarbons (PAHs) was determined and it was noted that the concentration of PAHs with more than 4 rings were increased. The source origin of the PAHs was investigated by use of relative ratios of PAH isomers and indicated that some formation of PAHs was additionally taking place during burning. © 2012 Elsevier Ltd.
Creep measurements confirm steady flow after stress maximum in extension of branched polymer melts

We provide conclusive evidence of nonmonotonic mechanical behavior in the extension of long-chain branched polymer melts. While nonmonotonic behavior is known to occur for solids, for the case of polymeric melts, this phenomenon is in direct contrast with current theoretical models. We rule out the possibility of the overshoot being an experimental artifact by confirming the existence of steady flow after a maximum in the ratio of stress to strain rate versus strain under both constant stress and constant strain-rate kinematics. This observation indicates the omission of important physics from current models for these industrially important materials, whose processing properties depend on extreme molecular extension.

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Organisations: Department of Chemical and Biochemical Engineering, The Danish Polymer Centre, Center for Energy Resources Engineering, CERE – Center for Energy Resources Engineering
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Crystallization Kinetics within a Generic Modelling Framework

An existing generic modelling framework has been expanded with tools for kinetic model analysis. The analysis of kinetics is carried out within the framework where kinetic constitutive models are collected, analysed and utilized for the simulation of crystallization operations. A modelling procedure is proposed to gain the information of crystallization operation kinetic model analysis and utilize this for faster evaluation of crystallization operations.
Design of an Emulsion-based Personal Detergent through a Model-based Chemical Product Design Methodology

An extended systematic methodology for the design of emulsion-based Chemical products is presented. The methodology consists of a model-based framework involving seven sequential hierarchical steps: starting with the identification of the needs to be satisfied by the product and then adding one-by-one the different classes of chemicals, until a formulation is obtained, the stability of which as an emulsion is finally checked with appropriate models. Structured databases, appropriate pure component as well as mixture property models, rule-based selection criteria and CAMD techniques are employed together to obtain one or more candidate formulations. A conceptual casestudy representing a personal detergent is presented to highlight the methodology.

Design of a Tank Cleaning Blend through a Systematic Emulsified Product Design Methodology

Commercial and industrial detergents, formulated liquid blends, have recently become extremely sophisticated, in order to address a broad range of cleaning tasks and to deliver superior performances with a minimum of effort and time. These products, by definition, consist of different chemicals, each with a specific function related to the needs of the product: surfactants, builders, bleaching agents, enzymes and minors, usually mixed together with a carrier, necessary to keep the blend as a homogeneous liquid formulation. A system approach and associated tools can help to virtually generate and test different candidates in order to identify the most promising formulations before a detailed
Prediction of properties is important in chemical process-product design. Reliable property models are needed for increasingly complex and wider range of chemicals. Group-contribution methods provide useful tool but there is a need to validate them and improve their accuracy when complex chemicals are present in the mixtures. In accordance with that, a combined group-contribution and atom connectivity approach that is able to extend the application range of property models has been developed for mixture properties. This so-called Group-ContributiorPlus (GCPlus) approach is a hybrid model which combines group contribution and molecular descriptor theories (such as connectivity indices – CI). Connectivity indices are formalisms defined via graph theoretical concepts intended to describe the topological characteristics of molecular structures. The main idea is the use of connectivity indices to describe the molecular fragmentation that relates properties which is the molecular interactions with the molecular structures. One well known and established group-contribution method is the UNIFAC model, used to predict liquid phase activity coefficients for mixtures. The needed values of the group interaction parameters (GIPs) are obtained by fitting phase equilibrium data. There are, however many gaps in the UNIFAC parameter table due to lack of data. Alternative to performing measurements, which may not be feasible, values of the missing GIPs, can be predicted through the GCPlus approach. The predicted values for the GIPs are then used in the UNIFAC model to calculate activity coefficients. This approach can increase the application range of any “host” UNIFAC model by providing a reliable predictive model towards fast and efficient product
This PhD project is focused on the analysis and further development of the GCPlus approach for predicting mixture properties to be called the UNIFAC-CI model. The contributions of this work include an analysis of the developed Original UNIFAC-CI model in order to investigate why the model does not perform as well as the reference UNIFAC model for some systems while performing surprisingly better than the reference model for other systems. In this analysis, it is found that by introducing more structural information to the CHO group through the valence connectivity index (CI), the correlation error involving alkanes-aldehydes system can be reduced. This work is presented in Chapter 3. Furthermore in Chapter 4, as a continuation of the analysis done for systems involving C, H and O atoms, the Original UNIFAC-CI (VLE) model has been further reused and significantly expanded by including nitrogenated, chlorinated and sulfurated systems and the involved atom interaction parameters (AIPs) have been regressed. In addition to that, another set of parameters have been generated for the Original UNIFAC-CI (VLE) model using a quality assessment algorithm, QVLE (combination of 4 VLE consistency tests) as a weighting factor for each VLE dataset in the objective function for regression of AIPs. The quality factors are useful in identifying anomalous systems which can be problematic in the parameter estimation and can produce parameters which are not accurately representing the systems used for the regression. Moreover, in Chapter 5 the Original UNIFAC-CI (VLE/SLE) model have been developed where the atom interaction parameters (AIPs) are obtained through regression against both VLE and SLE experimental data. The prediction accuracy of SLE systems using the regressed parameters has been slightly increased. Besides that, in Chapter 6, Modified (Dortmund) UNIFAC-CI has been further developed by including chlorinated and sulfurated VLE systems. Finally, in Chapter 7, the developed Original UNIFAC-CI (VLE/SLE) model has been highlighted in selected case studies involving the design of a working solution for hydrogen peroxide production and solubility investigation of pharmaceutical systems where new group have been created and their interaction parameters are predicted/fine tuned generating a master parameter table specifically for those case studies. Also, the applicability of the Original UNIFACCI model is shown for predicting phase equilibria of lipid systems, filling missing GIPs and improving prediction of azeotropic mixture. In Chapter 8, a discussion with concluding remarks and recommendation for future work are presented.
Development of a New Comprehensive Framework for Surfactant Selection and Design for Emulsion-based Chemical Product Design

General information
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Development of corresponding states model for estimation of the surface tension of chemical compounds
The gene expression programming (GEP) strategy is applied for presenting two corresponding states models to represent/predict the surface tension of about 1,700 compounds (mostly organic) from 75 chemical families at various temperatures collected from the DIPPR 801 database. The models parameters include critical temperature or temperature/critical volume/acentric factor/critical pressure/reduced temperature/reduced normal boiling point temperature/molecular weight of the compounds. Around 1,300 surface tension data of 118 random compounds are used for developing the first model (a four-parameter model) and about 20,000 data related to around 1,600 compounds are applied for checking its prediction capability. For the second one (a five-parameter model), about 10,000 random data are applied for its development, and 11,000 data are used for testing its prediction ability. The statistical parameters including average absolute relative deviations of the results form dataset values (25 and 18% for the first and second models, respectively) demonstrate the accuracy of the presented models. © 2012 American Institute of Chemical Engineers AIChE J, 59: 613–621, 2013

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Web of Science (2002): Indexed yes
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10.1002/aic.13824
Dipolar cross-linkers for PDMS networks with enhanced dielectric permittivity and low dielectric loss

Dipole grafted cross-linkers were utilized to prepare polydimethylsiloxane (PDMS) elastomers with various chain lengths and with various concentrations of functional cross-linker. The grafted cross-linkers were prepared by reaction of two alkyne-functional dipoles, 1-ethynyl-4-nitrobenzene and 3-((4-nitrophenyl)diazenyl)phenoxy)-prop-1-yn-1-ylium, with a synthesized silicone compatible azide-functional cross-linker by click chemistry. The thermal, mechanical and electromechanical properties were investigated for PDMS films with 0 to 3.6 wt% of dipole-cross-linker. The relative dielectric permittivity was found to increase by ~20% at only 0.46 wt% of incorporated dipole without significant changes in the mechanical properties. Furthermore, the dielectric losses were proved to be remarkably low while the electrical breakdown strengths were high.
Distribution of MEG and methanol in well-defined hydrocarbon and water systems: Experimental measurement and modeling using the CPA EoS

Liquid-liquid equilibria data for two binary and two ternary systems are reported in the temperature range of 303.15-323.15 K at atmospheric pressure. The binary systems measured are n-nonane + MEG and ethylbenzene + MEG and the ternary systems are n-nonane + MEG + water and ethylbenzene + MEG + water. These data are satisfactorily correlated (binaries) and predicted (ternaries) using Cubic Plus Association (CPA) equation of state (EoS). CPA is also applied to binary LLE of aromatic hydrocarbon + water and VLE of methane + methanol. Finally the distribution of water and inhibitors (methanol and MEG) in various phases is modeled using CPA. The hydrocarbon phase consists of mixture-1 (methane, ethane, n-butane) or mixture-2 (methane, ethane, propane, n-butane, n-heptane, toluene and n-decane). CPA can satisfactorily predict the water content in the gas phase of the multicomponent systems containing mixture-1 over a range of temperatures and pressures. Similarly the methanol content in the gas phase of mixture-1 + water + methanol systems is predicted satisfactorily with accuracy within experimental uncertainty. For VLLE of mixture-2 + mixture-2 + MEG + water and mixture-2 + methanol + water systems, the organic phase compositions are satisfactorily predicted whereas modeling results are relatively less satisfactory for the vapor phase compositions partially due to uncertainties in the experimental data. © 2012 Elsevier B.V.

General information
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Main Research Area: Technical/natural sciences
Dual Decomposition for Large-Scale Power Balancing

Dual decomposition is applied to power balancing of exible thermal storage units. The centralized large-scale problem is decomposed into smaller subproblems and solved locally by each unit in the Smart Grid. Convergence is achieved by coordinating the units consumption through a negotiation procedure with the dual variables.

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Early Termination of Dantzig-Wolfe Algorithm for Economic MPC

In this paper we apply the Economic Model Predictive Control (MPC) for balancing the power supply and demand in the future power systems in the most economic way. The control problem is formulated as a linear program, having a block-angular structure solved by the implementation of the Dantzig-Wolfe decomposition. For real-time applications we introduce an early termination technique. Simulations demonstrate that the algorithm developed operates efficiently a power system, reducing significantly computational time.

General information
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Efficient Implementation of the Riccati Recursion for Solving Linear-Quadratic Control Problems

In both Active-Set (AS) and Interior-Point (IP) algorithms for Model Predictive Control (MPC), sub-problems in the form of linear-quadratic (LQ) control problems need to be solved at each iteration. The solution of these sub-problems is typically the main computational effort at each iteration. In this paper, we compare a number of solvers for an extended formulation of the LQ control problem: a Riccati recursion based solver can be considered the best choice for the general problem with dense matrices. Furthermore, we present a novel version of the Riccati solver, that makes use of the Cholesky factorization of the Pn matrices to reduce the number of flops. When combined with regularization and mixed precision, this algorithm can solve large instances of the LQ control problem up to 3 times faster than the classical Riccati solver.

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Electromechanically active polymer transducers: research in Europe

Smart materials and structures based on electromechanically active polymers (EAPs) represent a fast growing and stimulating field of research and development. EAPs are materials capable of changing dimensions and/or shape in response to suitable electrical stimuli. They are commonly classified in two major families: ionic EAPs (activated by an electrically induced transport of ions and/or solvent) and electronic EAPs (activated by electrostatic forces).

These polymers show interesting properties, such as sizable active strains and/or stresses in response to electrical driving, high mechanical flexibility, low density, structural simplicity, ease of processing and scalability, no acoustic noise and, in most cases, low costs.

Since many of these characteristics can also describe natural muscle tissues from an engineering standpoint, it is not surprising that EAP transducers are sometimes also referred to as 'muscle-like smart materials' or 'artificial muscles'. They are used not only to generate motion, but also to sense or harvest energy from it. In particular, EAP electromechanical transducers are studied for applications that can benefit from their 'biomimetic' characteristics, with possible usages from the micro- to the macro-scale, spanning several disciplines, such as mechatronics, robotics, automation, biotechnology and biomedical engineering, haptics, fluidics, optics and acoustics.

Currently, the EAP field is just undergoing its initial transition from academic research into commercialization, with companies starting to invest in this technology and the first products appearing on the market.

This focus issue is intentionally aimed at gathering contributions from the most influential European groups working in the EAP field. In fact, today Europe hosts the broadest EAP community worldwide. The rapid expansion of the EAP field in Europe, where it historically has strong roots, has stimulated the creation of the 'European Scientific Network for Artificial Muscles—ESNAM', entirely focused on EAPs and gathering the most active research institutes, as well as key industrial developers and end users. The ESNAM network has received financial support from the European COST (Cooperation in Science and Technology) programme (COST Action MP1003), leading to fruitful collaboration, of which some results are showcased in this issue.

This focus issue deals with a number of relevant topics on ionic and electronic EAPs. The contents, which span highly heterogeneous and cross diverse disciplines, such as physics, chemistry, material science and engineering, embrace size scales from nano to macro, and cover different areas, such as new materials, devices and applications.

This collection of papers helps elucidate, on the one hand, how heterogeneous and dynamic the EAP field is in general and, on the other hand, the state of the art of the EAP research in Europe.

We hope that this focus issue might help to stimulate future work in this emerging field of research and generate new applications.
Equilibrium Solubility of CO2 in Alkanolamines

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Evaluation of the PC-SAFT, SAFT and CPA equations of state in predicting derivative properties of selected non-polar and hydrogen-bonding compounds

In order to provide a comprehensive understanding of the potential and limitations of the PC-SAFT, SAFT and CPA equations-of-state, this study offers insight into their application for the prediction of derivative properties over extensive ranges of pressure and temperature. The ability of these models to predict selected properties (heat capacities, pressure-volume derivative, pressure-temperature derivative and speed of sound) are evaluated for n-alkanes and 1-alkohols. For n-alkanes, it is shown that the cubic term of CPA is unable to describe the pressure-volume derivative at high pressures, which is a major shortcoming in predicting derivative properties compared to SAFT-based models. Although PC-SAFT and SAFT provide a substantially better prediction of the pressure-volume derivative than CPA, they are still not accurate enough to obtain good speed of sound predictions. All three models are unable to accurately correlate the isochoric heat capacity, indicating an incorrect temperature dependency in these models. PC-SAFT shows peculiar behaviour in the description of the isobaric heat capacity of alkanes that can be traced back to the incorrect description of the pressure-temperature derivative. For 1-alkohols, both CPA and PC-SAFT accurately predict the isobaric heat capacity when modelled with the 3B association scheme, while SAFT is unable to capture the singularities present in the property irrespective of the association scheme used. None of the models are able to predict the speed of sound accurately, because the terms describing physical interactions result in poor estimates of the pressure-volume derivative that governs the property. © 2012 Elsevier B.V.

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Scopus rating (2009): SJR 1.133 SNIP 1.164
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.227 SNIP 1.09
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.031 SNIP 1.151
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.034 SNIP 1.245
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.009 SNIP 1.3
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 0.985 SNIP 1.349
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 1.193 SNIP 1.301
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 0.722 SNIP 1.101
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 0.966 SNIP 1.284
Web of Science (2001): Indexed yes
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Web of Science (2000): Indexed yes
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Exercise effects in a virtual type 1 diabetes patient: Using stochastic differential equations for model extension

The use of virtual patients for in silico testing of control algorithms for an artificial pancreas is growing. It is an easy, fast and low-cost alternative to pre-clinical testing. To simulate the everyday life of a type 1 diabetes (T1D) patient a simulator must be able to take into account physical activity. Exercise constitutes a substantial challenge to closed-loop control of T1D. The effects are many and depend on intensity and duration and may be delayed by several hours. In this study, we use a model for the glucoregulatory system based on the minimal model and a previously published extension incorporating exercise effects on insulin and glucose dynamics. Our model is constructed as a stochastic state space model consisting of a set of stochastic differential equations (SDEs). In a stochastic state space model, the residual error is split into random measurement error and misspecification noise. The latter of the two can be used to pinpoint model deficiencies or unknown influential factors during the development of the model. The model is thus built on the basis of physiological knowledge of the system combined with information from observed data. Model parameters are estimated on clinical data from a study including exercise bouts of 20 minutes performed on 12 T1D patients treated with continuous subcutaneous insulin infusion. The predictive abilities of the model are investigated. In conclusion, this study illustrates the advantages of using SDEs in the development of an extended glucoregulatory model including effects of exercise suited for in silico testing.

General information

State: Published
Organisations: Department of Applied Mathematics and Computer Science, Center for Energy Resources Engineering, Scientific Computing, Dynamical Systems, Copenhagen University Hospital
Authors: Duun-Henriksen, A. K. (Intern), Schmidt, S. (Ekstern), Nørgaard, K. (Ekstern), Jørgensen, J. B. (Intern), Madsen, H. (Intern)
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BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.223 SNIP 1.035 CiteScore 1.52
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.315 SNIP 1.14 CiteScore 2.09
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
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Experimental determination and modeling of the phase behavior for the direct synthesis of dimethyl carbonate from methanol and carbon dioxide

This study focuses on the investigation of the phase behavior of mixtures relevant to the direct synthesis of dimethyl carbonate from methanol and carbon dioxide. The bubble points of corresponding quaternary mixtures of varying composition were experimentally determined. The Cubic-Plus-Association (CPA) equation of state was applied to model the phase behavior of the experimentally studied systems. In this regard, the CPA binary interaction parameters were estimated based on experimental data for the corresponding binary systems available in the literature, and subsequently the model was applied to predict the phase behavior of the multicomponent systems. It was shown that CPA is capable of predicting the phase behavior of such complex systems containing polar and associating components at high temperatures and pressures with reasonable accuracy considering the non-ideality of such mixtures. The results reveal P–T regions where the system can exist in one single phase and where it is multiphase, which can be used for further optimization not only of the chemical reaction itself but also subsequent product separation processes.

General information
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Organisations: Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering, Center for Energy Resources Engineering, CHEC Research Centre, Swiss Federal Institute of Technology
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Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.921 SNIP 1.216 CiteScore 2.71
Factors Impacting the Conversion of Abstracts Presented at the Canadian Cardiovascular Congress Meetings to Full Publications

Objective: We sought to determine the rate of conversion of scientific abstracts presented at the Canadian Cardiovascular Conference (CCC), between 2006 and 2008, into peer reviewed manuscript publications within two years of their initial presentation. Moreover, we sought to identify factors associated with transition of abstracts to full publications.

Background: The rate of conversion of abstracts presented at scientific meetings into peer reviewed published manuscripts, has been a topic of interest for various medical specialties. Rapid translation of abstracts into manuscripts allows for reliable and rapid communication of scientific knowledge into practice.

Methods: Using a previously validated automated computer algorithm, we searched the ISI Web of Science to identify peer-reviewed full manuscript publications of abstracts presented at the CCC. We manually entered information about abstracts presented in the CCC between 2006 and 2010, including data on the type of presentation (oral vs poster), category (basic science vs clinical cardiology) and the number of authors. Publication rates, mean time to publication, the mean number of citations and mean journal impact factor were determined.

Results: From 2006 to 2010, 3665 abstracts were presented at the CCC. Overall 24% of presented abstracts were published within 2 years of the conference. Mean impact factor for publications was 5.2 (range 0.4-53.2). Mean citations for published manuscripts was 14.4 (range 0-483). Of the abstracts that were eventually published, 4% publications were in the Canadian Journal of Cardiology. Mean duration from abstract presentation at CCC
to full manuscript publication was 13 months. Conclusion: Publication rates of presented abstracts at the CCC (24%) is lower than that reported for abstracts presented at American College of Cardiology (ACC) (29.5%), American Heart Association (AHA) (34.5%) and European Society of Cardiology (ESC) (27%). This highlights the need to identify factors associated with improved abstract publication - this is an area of ongoing research for our group. Copyright © 2013 Published by Elsevier Inc.
Fluid phase equilibria during propylene carbonate synthesis from propylene oxide in carbon dioxide medium

In the present study the influence of the amount of carbon dioxide on the catalytic performance during the propylene carbonate synthesis from propylene oxide and CO2 was investigated. The reaction was performed in high-pressure batch autoclaves using immobilized 1-hydroxyethyl-9-propyl-cyclic guanidinium bromide on SBA-15 (HEPCGBr/SBA-15) as catalyst in the absence of any co-catalyst. It was found that the yield was strongly dependent on the amount of CO2 added to the system and that the phase behavior strongly changes along the reaction pathway. The Cubic-Plus-Association (CPA) equation of state was used to predict the phase behavior during the reaction and the number and composition of coexisting phases in the multicomponent reaction system were determined. In accordance with the experimental data, the maximum conversion was achieved in the transition region between the two- and the one-phase region where a CO2-expanded reactant/product phase (larger volume due to the dissolution of carbon dioxide in the liquid phase) is present. Optimal conditions for performing the reaction have been derived which requires consideration not only of the phase behavior of the starting phase but also of the mixture during reaction. © 2013 Elsevier B.V. All rights reserved.
Freezing Point Depressions of Phase Change CO2 Solvents

Freezing point depressions (FPD) in phase change solvents containing 2-(diethylamino)ethanol (DEEA) and 3-(methylamino)propylamine (MAPA) were measured using a modified Beckmann apparatus. The measurements were performed for the binary aqueous DEEA and MAPA solutions, respectively, in the concentration ranges of (0 to 55) mass percent and (0 to 32.5) mass percent of amine. For the ternary aqueous DEEA–MAPA solutions, freezing points were measured for 5:1, 3:1, 1:1, 1:3, and 1:5 molar ratios of DEEA/MAPA. The FPD method was extended for easy and accurate measurement of freezing points in the CO2 loaded systems. It is based on saturation of the solution by CO2 and then dilution by using a batch of the original unloaded solution in order to get the solutions with different CO2 loadings. Freezing point measurements were then carried out for (12, 20, 30, and 33) mass percent DEEA solutions and (10, 20, and 27) mass percent MAPA solutions at different CO2 loadings. The apparatus and the experimental method used showed good repeatability and accuracy. The measured freezing point data were compared with monoethanolamine (MEA) and methyl diethanolamine (MDEA) found in the literature. The experimental values indicate that the DEEA–water interaction is almost similar to that of MEA–water interaction. MAPA has shown a stronger nonideal behavior compared to DEEA. A correlation for the freezing points as a function of solution composition was formulated for the unloaded binary and ternary systems.

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<td>2</td>
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Original language: English

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Relations
GC-PPC-SAFT equation of state for VLE and LLE of hydrocarbons and oxygenated compounds. Sensitivity analysis

Group-contribution polar versions of SAFT equations of state are very useful for predictive calculations of mixtures containing diverse polar molecules. In this work, we have evaluated the predictive performance of one such model, the so-called polar perturbed-chain (PPC) SAFT model for phase-equilibrium properties of 290 hydrocarbons and monofunctional oxygenated compounds. Emphasis has been given on carrying out an extensive evaluation considering diverse types of phase behavior (vapor-liquid and liquid-liquid equilibria) and properties/conditions (Henry's law constant for H2, N2, and CH4; infinite-dilution activity coefficient in water; solubility in water; infinite-dilution n-octanol/water partition coefficient). In general, considering the predictive nature of the calculations, encouraging results were obtained. For pure-component vapor pressures and liquid molar volumes, the deviations are very small, at 20% and 3%, respectively. The deviations in the prediction of the Henry's law constants are within a factor of 2, with the best results found for the methane and nitrogen solubilities. For solubilities in water and, consequently, for infinite-dilution n-octanol/water partition coefficients, deviations are within a factor of 2 for hydrocarbons and within a factor of 4 for alcohols and aldehydes, but they are large for the other oxygenated families. To identify paths for improvement, a sensitivity analysis was performed, indicating that all of the parameters make large contributions to almost all properties. In addition, the sensitivity of the infinite-dilution activity coefficient in water to the molecular size parameters was extremely high. This suggests that a small change in these parameters might improve the results significantly. © 2013 American Chemical Society.
Heat of Absorption of CO2 in Aqueous Solutions of DEEA, MAPA and their Mixture

A reaction calorimeter was used to measure the differential heat of absorption of CO2 in phase change solvents as a function of temperature, CO2 loading and solvent composition. The measurements were taken for aqueous solutions of 2-(diethylamino)ethanol (DEEA), 3-(methylamino)propylamine (MAPA) and their mixture. The tested compositions were 5M DEEA, 2M MAPA and their mixture, 5M DEEA + 2M MAPA which gives two liquid phases on reacting with CO2. Experimental measurements were also carried out for 30% MEA used as a base case. The measurements were taken isothermally at three different temperatures 40, 80 and 120°C at a CO2 feed pressure of 600kPa. In single aqueous amine solutions, heat of absorption increases with increase in temperature and depends on the type of amine used. DEEA, a tertiary amine, has lower heat of absorption compared to MAPA being a diamine with primary and secondary amine functional groups. For amine mixtures, heat of absorption is a function of CO2 loading and temperature. The heat of absorption against CO2 loading depends on the composition of the amines in the mixture. All the measured data in this work were compared with 30% MEA at absorption (40°C) and desorption (120°C) conditions.

General information
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Organisations: Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering, Norwegian University of Science and Technology
Authors: Waseem Arshad, M. (Intern), von Solms, N. (Intern), Thomsen, K. (Intern), Svendsen, H. F. (Ekstern)
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Heat of Absorption of CO2 in Phase Change Solvents: 2-(Diethylamino)ethanol and 3-(Methylamino)propylamine

Heat of absorption of CO2 in phase change solvents containing 2-(diethylamino)ethanol (DEEA) and 3-(methylamino)propylamine (MAPA) were measured as a function of CO2 loading at different temperatures using a commercially available reaction calorimeter. The tested systems were aqueous single amines (5 M DEEA, 2 M MAPA, and 1 M MAPA) and aqueous amine mixtures (5 M DEEA + 2 M MAPA and 5 M DEEA + 1 M MAPA) which give two liquid phases on reacting with CO2. All parallel experiments have shown good repeatability. The measurements were taken isothermally at three different temperatures, (40, 80, and 120) °C. The measured differential heat of absorption values were converted into integral values by integration. Heats of absorption of CO2 in aqueous single amines were affected by changing the solvent composition (large difference in concentrations) and CO2 feed pressure simultaneously. In addition to these two parameters, it also depends on temperature and the type of amine used. Tertiary alkanolamine (DEEA) has shown greater dependency on these parameters compared to the diamine (MAPA) containing both primary and secondary amine functional groups. In aqueous amine mixtures, heats of absorption depend on CO2 loading, temperature, and composition of the constituent amines in the mixture. All measured heat of absorption data were compared with 30 mass % MEA used as a base case.
Heterogeneously Catalysed Chemical Reactions in Carbon Dioxide Medium

In this PhD-study the different areas of chemical engineering, heterogeneous catalysis, supercritical fluids, and phase equilibrium thermodynamics have been brought together for selected reactions. To exploit the beneficial properties of supercritical fluids in heterogeneous catalysis, experimental studies of catalytic chemical reactions in dense and supercritical carbon dioxide have been complemented by the theoretical calculations of phase equilibria using advanced thermodynamic models.

In the recent years, the use of compressed carbon dioxide as innovative, non-toxic and non-flammable, cheap, and widely available reaction medium for many practical and industrial applications has drastically increased. Particularly attractive are heterogeneously catalysed chemical reactions. The beneficial use of CO2 is attributed to its unique properties at dense and supercritical states (at temperatures and pressures above the critical ones), i.e. when it combines both gas-like and liquid-like properties. In terms of practical use it means that CO2 can be used as an effective solvent for reactants, while the viscosity and diffusion coefficients are close to those for gases, which minimises heat and mass transport limitations in case of heterogeneous catalysis.

Previous reports and the studies in the present thesis have shown that phase behaviour can play a crucial role in chemical reactions, especially when they are performed near the supercritical region of the reaction mixture. Experimental monitoring and determination of phase equilibria is very time consuming, expensive, and very often reveals very little information. However, these problems can be overcome when thermodynamic modelling is applied. The Cubic-Plus-Association Equation of State (CPA) was used throughout this study; therefore this model is discussed more extensively. Heterogeneously catalysed hydrogenation reactions are considered to be quite well studied and established. However, the catalyst performance can alter significantly when the reaction is performed in carbon dioxide medium. This effect was studied with the example of the selective hydrogenation of 2-butenal over palladium catalyst. It was found that the maximum conversion of 2-butenal is achieved when the reaction mixture exists in the near-critical region, or the so-called “expanded-liquid” phase. Some possible reasons for that have been proposed.

Aldol reactions are the complex processes that are very important for the chemical industry. Furthermore, multistep reactions performed in “one-pot” using multifunctional catalysts attract a lot of interest. Thus, a part of this thesis was devoted to performing the aldol reaction and the “one-pot” synthesis of aldol products starting from the selective hydrogenation of unsaturated aldehydes in carbon dioxide medium. It was found that supported tungstosilicic acid catalysts and acidic resin Amberlyst-15 are very effective for performing aldol reactions. The positive influence of temperature and CO2-content on catalyst activity was studied. Furthermore, the “one-pot” synthesis with 2-butenal was performed using bifunctional and mixed catalysts. The reactions were studied in different reactor types and reaction conditions were optimised using CPA calculations. Extensive catalyst characterisation was carried out in order to understand the catalyst structure.

Carbon dioxide can play a dual role in some chemical reactions, i.e. as reaction medium and as one of the reactants. An example of this reaction is the synthesis of propylene carbonate from propylene oxide and CO2. The study of the phase equilibrium in this case is more complex not only because the composition changes due to the chemical reaction, but also due to the constantly decreasing amount of solvent. Furthermore, organic carbonates have significantly lower solubility in CO2 than reacting epoxides. In this part of the study, the influence of CO2-content on the performance of the immobilized 1-hydroxyethyl-9-propyl-cyclguanidinium bromide on SBA-15 (HEPCGBr/SBA-15) catalyst was investigated. The maximum conversion was observed in the transition region from the two- to one-phase state. This finding was supported by previous experimental studies. Thermodynamic calculations were shown to be extremely useful for the phase behaviour investigations.

The direct synthesis of dimethyl carbonate from methanol and CO2 has been investigated for quite a long time, however hardly any sufficiently active catalysts have been found so far. Nevertheless, optimisation of the phase equilibria of the reaction mixture can make the process economically more feasible. Many different thermodynamic models of different capability and applicability have been applied for this task. The CPA model is an advanced model that accounts for complex interactions between associating molecules like water and methanol. It has been shown that CPA can satisfactorily describe any type of phase equilibria for the quaternary reaction mixture as well as ternaries and binaries that comprise it. This makes CPA a universal and very useful model for many practical applications.

All aforementioned studies have shown that supercritical fluids in heterogeneous catalysis complemented by thermodynamic modelling have an immense potential for further investigations.
High dielectric permittivity elastomers from well-dispersed expanded graphite in low concentrations

The development of elastomer materials with a high dielectric permittivity has attracted increased interest over the last years due to their use in for example dielectric electroactive polymers. For this particular use, both the electrically insulating properties - as well as the mechanical properties of the elastomer - have to be tightly controlled in order not to destroy favorable elastic properties by the addition of particles. In the following, expanded graphite in low concentrations (up to 5 wt%) are investigated as a possible candidate as filler materials in very soft elastomers, which by the addition of traditional fillers in the necessary amounts would either lose their stability or their softness. Furthermore the influence of several mixing procedures on the electrical and mechanical properties is investigated. © 2013 SPIE.

General information

State: Published
Organisations: Department of Chemical and Biochemical Engineering, The Danish Polymer Centre, Center for Energy Resources Engineering
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Hot embossing of microstructures on addition curing polydimethylsiloxane films

The aim of this research work is to establish a hot embossing process for addition curing vinyl-terminated polydimethylsiloxane (PDMS), which are thermosetting elastomers, based on the existing and widely applied technology for thermoplasts. To our knowledge, no known technologies or processes are commercially available for embossing microstructures and submicron structures on elastomers like silicones in large scale production of films. The predominantly used technologies to make microscale components for microfluidic devices and microstructures on PDMS elastomer is (a) reaction injection molding, (b) ultraviolet lithography, and (c) photolithography. We focus on hot embossing as it is one of the simplest, most cost-effective, and time-saving methods for replicating structures for thermoplasts. Addition curing silicones are shown to possess the ability to capture and retain an imprint made on it, 10–15 min after the gel point at room temperature. This property is exploited in the hot embossing technology.
Hot-embossing of microstructures on addition-curing polydimethylsiloxane films
To our knowledge no known technologies or processes are commercially available for embossing microstructures and sub-micron structures on elastomers like silicones in large scale production of films. The predominantly used technologies to make micro-scale components for micro-fluidic devices and microstructures on PDMS elastomer are 1) reaction injection molding 2) UV lithography and 3) photolithography, which all are time-consuming and not suitable for large scale productions. A hot-embossing process to impart micro-scale corrugations on an addition curing vinyl terminated PDMS (polydimethyl siloxane) film, which is thermosetting elastomer, was established based on the existing and widely applied technology for thermoplasts. We focus on hot-embossing as it is one of the simplest, most cost-effective and time saving methods for replicating structures for thermoplasts. Addition curing silicones are shown to possess the ability to capture and retain an imprint made on it 10-15 minutes after the gel-point at room temperature. This property is exploited in the hot-embossing technology. © 2013 SPIE.

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Conducting polymers, Curing, Elastomers, Electroactive polymer actuators, Microchannels, Microstructure, Photolithography, Plastic films, Reaction injection molding, Technology, Thermosets, Silicones
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Improved population balance model for straining-dominant deep bed filtration using network calculations
Colloidal-suspension flow in porous media is modelled simultaneously by the large scale population balance equations and by the microscale network model. The phenomenological parameter of the correlation length in the population balance model is determined from the network modelling. It is found out that the correlation length in the population balance model depends on the particle size. This dependency calculated by two-dimensional network has the same tendency as that obtained from the laboratory tests in engineered porous media.

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Organisations: Center for Energy Resources Engineering, CERE – Center for Energy Ressources Engineering, Department of Chemical and Biochemical Engineering, University of Adelaide
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Intelligente materialer som kunstige muskler og energi-høstere

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Organisations: Department of Chemical and Biochemical Engineering, The Danish Polymer Centre, Center for Energy Resources Engineering
Authors: Bahrt, F. (Intern), Daugaard, A. E. (Intern), Hvilsted, S. (Intern), Skov, A. L. (Intern)
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Inverse Problems in Geosciences: Modelling the Rock Properties of an Oil Reservoir

Even the most optimistic forecasts predict that Danish oil production will decrease by 80% in the period between 2006 and 2040, and only a strong innovative technological effort can change that. Due to the geological structures of the subsurface in the Danish part of the North Sea, Denmark is currently missing out on approximately 70% of the oil, which is left behind, trapped in unreachable parts of the reservoirs.

An increase in the oil recovery rate can be achieved by better planning and optimisation of oil production. Both require an improved description of the rock properties of the subsurface of the reservoirs. Hence the focus of this work has been on acquiring models of spatial parameters describing rock properties of the subsurface using geostatistical a priori knowledge and available geophysical data. Such models are solutions to often severely under-determined, inverse problems.

The focus of the study has been on the computational aspects of inferring such models. Reservoir modelling is a large-scale problem with great computational complexity and the work should be seen as a first part of a foundation for one day, when the computational resources are available, being able to handle the large scale problems of the petroleum industry. But for now most of the study is based on simplified and idealised models.

We have proposed a method for efficient and accurate interpolation of rock properties from seismic data. It is based on a recently published paper on interpolation of rock properties that breaks with the dominating influence of spatial coordinates in traditional interpolation methods. The thesis contains work involving a test case study of the method demonstrating how the interpolation in attribute space ensures the geological structures of the computed models and how the method can be further improved by an orthogonal transformation of the attribute space.

We have formulated a closed form expression of an a priori probability density function that quantifies the statistical probability of models describing the rock properties of a reservoir. This can be used to evaluate the probability that a model adhere to prior knowledge by having specific multiple-point statistics, for instance, learned from a training image. Existing methods efficiently sample an a priori probability density function to create a set of acceptable models; but they cannot evaluate the probability of a model.

We have developed and implemented the Frequency Matching method that uses the closed form expression of the a priori probability density function to formulate an inverse problem and compute the maximum a posteriori solution to it. Other methods for computing models that simultaneously fit data observations and honour a priori knowledge are not capable of computing the maximum a posteriori solution. Instead they either sample the posterior probability density function or they sample the a priori probability density function to optimise the likelihood function.

This thesis consists of a summary report and seven research papers submitted, reviewed and/or published in the period 2010 - 2013.
Inversion assuming weak scattering

The study of weak scattering from inhomogeneous media or interface roughness has long been of interest in sonar applications. In an acoustic backscattering model of a stationary field of volume inhomogeneities, a stochastic description of the field is more useful than a deterministic description due to the complex nature of the field. A method based on linear inversion is employed to infer information about the statistical properties of the scattering field from the obtained cross-spectral matrix. A synthetic example based on an active high-frequency sonar demonstrates that the proposed method provides a quantitative description of a weak scattering field in terms of its second-order statistics.

General information
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Weak scattering, Least-squares inversion, High-frequency active sonar, Covariance matrix
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Investigation of Kinetic Hydrate Inhibition Using a High Pressure Micro Differential Scanning Calorimeter

Methane hydrate formation and decomposition were investigated in the presence of the kinetic inhibitor (Luvicap EG) and synergist (polyethylene oxide; PEO) using a high pressure micro-differential scanning calorimeter (HP-μDSC) with both temperature ramping and isothermal temperature programs. These investigations were performed using small samples in four different capillary tubes in the calorimeter cell. When the isothermal method was employed, it was found that Luvicap EG significantly delays the hydrate nucleation time as compared to water. The results obtained from the ramping method demonstrated that in the presence of Luvicap EG hydrate nucleation temperature was reduced. However, the presence of Luvicap EG promoted the extent of hydrate formation once nucleation had occurred. The addition of a small amount of PEO enhanced the nucleation inhibition capability of Luvicap EG further and decreased the promotion of hydrate growth. Additionally, hydrate formed in the presence of inhibitor decomposed at higher temperatures compared to pure water, indicating that while hydrate formation is initially inhibited; once hydrates form, they are more stable in the presence of inhibitor. Overall, this method proved a viable experimental technique, especially in the case of screening expensive and rarely available materials, such as biologically based inhibitors, before scale up.

General information
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Organisations: Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering
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Web of Science (2018): Indexed yes
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Web of Science (2017): Indexed yes
Ionic networks derived from the protonation of dendritic amines with carboxylic acid end-functionalized PEGs

The synthesis and characterization of novel ionic networks linked by the ammonium salts of poly(propylene imine) (PPI) dendrimers of the first (PPI G1) and second (PPI G2) generation and two short bis carboxymethyl ether terminated poly(ethylene glycol)s (DiCOOH-PEG) with different molecular weights (Mn ~ 250 and Mn ~ 600) are reported. Likewise, an ionic network based on PPI G1 and a long αω-dicarboxylic acid functionalized PEG (Mn ~ 4800) were evaluated. Simpler ionic structures based on tris(2-aminoethyl)amine or hexamethylene diamine and the short DiCOOH-PEGs are also investigated. The ionic structures formed were confirmed by differential scanning calorimetry, Fourier Transform Infrared spectroscopy in the attenuated-total-reflection mode, and 1H-13C NMR spectroscopy. A comprehensive 1H NMR analysis revealed that only the primary amines of the PPI G1 dendrimer residing at the periphery take part in the ionic network formation. In the case of PPI G2, the picture is less clear. A thorough investigation of the thermal degradation of the utilized precursors and all the ionic materials prepared was additionally performed by thermogravimetric analysis. © 2012 Wiley Periodicals, Inc. J Polym Sci Part A: Polym Chem, 2013
Kaolinite Mobilisation in Sandstone: Pore Plugging vs. Suspended Particles

The effect of temperature and salinity on sandstone permeability is critical to the feasibility of heat storage in geothermal aquifers. Permeability reduction has been observed in Berea sandstone when the salinity of the pore water is reduced as well as when the sample is heated. Several authors suggest that this effect is due to kaolinite clay mobilisation from the quartz grain surface; the mobilised particles subsequently plug the pore throats and reduce the permeability irreversibly. The expected hysteresis is observed when the salinity is reduced and increased; however, in contradiction with the throat plugging theory, the effect of heating is found to be reversible with cooling. In laboratory experiments we heated Berea sandstone from 20°C to 80°C and observed a reversible permeability reduction. The permeability of the heated samples increased at higher flow rates. We propose that in this case the mobilised kaolinite particles either remain suspended and thereby increase the fluid viscosity, or form porous aggregates that can be destabilized by hydrodynamic forces. To address how the pore scale distribution of kaolinite relates to the permeability of the entire sample, we relate permeability to the effective specific surface, $S_p$. The effective specific surface represents the average surface area that resists the flow through the sample of a volume of fluid. We propose that flow paths with a small $S_p$ contribute more than proportionately to the total volume flux. Kaolinite mobilisation in pores with a small $S_p$ diverts fluid flow through pores with a higher $S_p$, and thereby reduces permeability of the entire sample.

In this paper, we use the DLVO theory to compare how temperature and salinity affect the surface interaction forces between quartz and kaolinite, as well as the interaction forces among kaolinite particles to evaluate whether heating can be expected to a) mobilise particles and b) result in kaolinite forming a suspension rather than plugging the pore throats.
Model-Based Closed-Loop Glucose Control in Type 1 Diabetes: The DiaCon Experience

Background:
To improve type 1 diabetes mellitus (T1DM) management, we developed a model predictive control (MPC) algorithm for closed-loop (CL) glucose control based on a linear second-order deterministic-stochastic model. The deterministic part of the model is specified by three patient-specific parameters: insulin sensitivity factor, insulin action time, and basal insulin infusion rate. The stochastic part is identical for all patients but identified from data from a single patient. Results of the first clinical feasibility test of the algorithm are presented.

Methods:
We conducted two randomized crossover studies. Study 1 compared CL with open-loop (OL) control. Study 2 compared glucose control after CL initiation in the euglycemic (CL-Eu) and hyperglycemic (CL-Hyper) ranges, respectively. Patients were studied from 22:00–07:00 on two separate nights.

Results:
Each study included six T1DM patients (hemoglobin A1c 7.2% ± 0.4%). In study 1, hypoglycemic events (plasma glucose < 54 mg/dl) occurred on two OL and one CL nights. Average glucose from 22:00–07:00 was 90 mg/dl [74–146 mg/dl; median (interquartile range)] during OL and 108 mg/dl (101–128 mg/dl) during CL (determined by continuous glucose monitoring). However, median time spent in the range 70–144 mg/dl was 67.9% (3.0–73.3%) during OL and 80.8% (70.5–89.7%) during CL. In study 2, there was one episode of hypoglycemia with plasma glucose <54 mg/dl in a CL-Eu night. Mean glucose from 22:00–07:00 and time spent in the range 70–144 mg/dl were 121 mg/dl (117–133 mg/dl) and 69.0% (30.7–77.9%) in CL-Eu and 149 mg/dl (140–193 mg/dl) and 48.2% (34.9–72.5%) in CL-Hyper, respectively.

Conclusions:
This study suggests that our novel MPC algorithm can safely and effectively control glucose overnight, also when CL control is initiated during hyperglycemia.

General information
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Organisations: Department of Applied Mathematics and Computer Science, Dynamical Systems, Center for Energy Resources Engineering, Scientific Computing, Copenhagen University Hospital
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BFI (2018): BFI-level 1
Model Identification Using Stochastic Differential Equation Grey-Box Models in Diabetes

BACKGROUND:
The acceptance of virtual preclinical testing of control algorithms is growing and thus also the need for robust and reliable models. Models based on ordinary differential equations (ODEs) can rarely be validated with standard statistical tools. Stochastic differential equations (SDEs) offer the possibility of building models that can be validated statistically and that are capable of predicting not only a realistic trajectory, but also the uncertainty of the prediction. In an SDE, the prediction error is split into two noise terms. This separation ensures that the errors are uncorrelated and provides the possibility to pinpoint model deficiencies.

METHODS:
An identifiable model of the glucoregulatory system in a type 1 diabetes mellitus (T1DM) patient is used as the basis for development of a stochastic-differential-equation-based grey-box model (SDE-GB). The parameters are estimated on clinical data from four T1DM patients. The optimal SDE-GB is determined from likelihood-ratio tests. Finally, parameter tracking is used to track the variation in the "time to peak of meal response" parameter.

RESULTS:
We found that the transformation of the ODE model into an SDE-GB resulted in a significant improvement in the prediction and uncorrelated errors. Tracking of the "peak time of meal absorption" parameter showed that the absorption rate varied according to meal type.

CONCLUSION:
This study shows the potential of using SDE-GBs in diabetes modeling. Improved model predictions were obtained due to the separation of the prediction error. SDE-GBs offer a solid framework for using statistical tools for model validation and model development.
Modeling of Dielectric Properties of Aqueous Salt Solutions with an Equation of State

The static permittivity is the most important physical property for thermodynamic models that account for the electrostatic interactions between ions. The measured static permittivity in mixtures containing electrolytes is reduced due to kinetic depolarization and reorientation of the dipoles in the electrical field surrounding ions. Kinetic depolarization may explain 25–75% of the observed decrease in the permittivity of solutions containing salts, but since this is a dynamic property, this effect should not be included in the thermodynamic modeling of electrolytes. Kinetic depolarization has, however, been ignored in relation to thermodynamic modeling, and authors have either neglected the effect of salts on permittivity or used empirical correlations fitted to the measured static permittivity, leading to an overestimation of the reduction in the thermodynamic static permittivity. We present a new methodology for obtaining the static permittivity over wide ranges of temperatures, pressures, and compositions for use within an equation of state for mixed solvents containing salts. The static permittivity is calculated from a new extension of the framework developed by Onsager, Kirkwood, and Fröhlich to associating mixtures. Wertheim’s association model as formulated in the statistical associating fluid theory is used to account for hydrogen-bonding molecules and ion–solvent association. Finally, we compare the Debye–Hückel Helmholtz energy obtained using an empirical model with the new physical model and show that the empirical models may introduce unphysical behavior in the equation of state.
Modeling of dielectric properties of complex fluids with an equation of state

The static permittivity is a key property for describing solutions containing polar and hydrogen bonding compounds. However, the precise relationship between the molecular and dielectric properties is not well-established. Here we show that the relative permittivity at zero frequency (static permittivity) can be modeled simultaneously with thermodynamic properties. The static permittivity is calculated from an extension of the framework developed by Onsager, Kirkwood, and Fröhlich to associating mixtures. The thermodynamic properties are calculated from the cubic-plus-association (CPA) equation of state that includes the Wertheim association model as formulated in the statistical associating fluid theory (SAFT) to account for hydrogen bonding molecules. We show that, by using a simple description of the geometry of the association, we may calculate the Kirkwood g-factor as a function of the probability of hydrogen bond formation. The results show that it is possible to predict the static permittivity of complex mixtures over wide temperature and pressure ranges from simple extensions of well-established theories simultaneously with the calculation of thermodynamic properties. © 2013 American Chemical Society.

General information
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BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.03 SJR 1.348 SNIP 1.02
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.367 SNIP 1.096 CiteScore 3.25
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.44 SNIP 1.14 CiteScore 3.28
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
A group-contribution (GC) property prediction model for estimating the critical micelle concentration (CMC) of nonionic surfactants in water at 25 °C is presented. The model is based on the Marrero and Gani GC method. A systematic analysis of the model performance against experimental data is carried out using data for a wide range of nonionic surfactants covering a wide range of molecular structures. As a result of this procedure, new third order groups based on the characteristic structures of nonionic surfactants are defined and are included in the Marrero and Gani GC model. In this way, those compounds that exhibit larger correlation errors (based only on first- and second-order groups) are assigned to more detailed molecular descriptions, so that better correlations of critical micelle concentrations are obtained. The group parameter estimation has been performed using a data set of 150 experimental measurements covering a large
variety of nonionic surfactants including linear, branched, and phenyl alkyl ethoxylates; alkanediols; alkyl mono- and disaccharide ethers and esters; ethoxylated alkyl amines and amides; fluorinated linear ethoxylates and amides; polyglycerol esters; and carbohydrate derivate ethers, esters, and thiols. The model developed consists of linear group contributions, and the critical micelle concentration is estimated using the molecular structure of the nonionic surfactant alone. Compared to other models used for the prediction of the critical micelle concentration, and in particular, the quantitative structure–property relationship models, the developed GC model provides an accurate correlation and allows for an easier and faster application in computer-aided molecular design techniques facilitating chemical process and product design.

General information
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Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.1 SJR 0.945 SNIP 1.139
Web of Science (2016): Indexed yes
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Scopus rating (2015): SJR 0.949 SNIP 1.146 CiteScore 2.87
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.012 SNIP 1.292 CiteScore 2.85
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 0.982 SNIP 1.243 CiteScore 2.6
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Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.066 SNIP 1.338 CiteScore 2.56
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.086 SNIP 1.24 CiteScore 2.58
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.047 SNIP 1.165
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.002 SNIP 1.164
Web of Science (2009): Indexed yes
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Scopus rating (2008): SJR 1.142 SNIP 1.267
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Scopus rating (2007): SJR 1.105 SNIP 1.239
Molasses injection as a MEOR strategy: Enrichment incubations of brine/oil from North Sea Oil Field

General information
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Number of pages: 1
Publication date: 2013
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Molecular Rheology of Complex Fluids
The processing of polymer materials is highly governed by its rheology, and influences the properties of the final product. For example, a recurring problem is instability in extrusion that leads to imperfect plastic parts. The ability to predict and control the rheological behavior of polymer fluids as a function of molecular chemistry has attracted a long history of collaboration between industry and academia. In industrial polymer processes, there is usually a combination of both shear and extensional flows. In some processing operations such as blow molding and fiber spinning, extensional flow is the dominant type of deformation. The polymer molecules experience a significant amount of chain orientation and stretching during these processes. Shear rheology measured by conventional shear rheometers is good at describing chain orientation, whereas extensional rheology gives a good way of inducing chain stretching. Accurate and reliable stress–strain measurements of extensional flow play a crucial role in the understanding of non-linear rheological properties of polymers. However, the non–linear extensional rheology has not been extensively studied. It is known that the rheology of polymer melts is highly sensitive to molecular architecture, but the precise connection between architecture and non–linear rheology is still not fully understood. For example, linear polymer melts have the simplest architecture, but the possible existence of a qualitative difference on extensional steady–state viscosity between melts and solutions is still an open question. Branched polymer melts have more complex molecular structures. A stress maximum during the start–up of uniaxial extensional flow was reported in 1979 for a low–density polyethylene (LDPE) melt. Subsequently observations of a steady stress following a stress maximum were reported for two LDPE melts. However the rheological significance of the stress maximum as well as the existence of steady flow conditions following the maximum is still a matter of some debate. This thesis focuses on the experimental study of extensional rheology of linear and branched polymer melts. We report the stress–strain measurements in extensional flows using a unique
Filament Stretching Rheometer (FSR) in controlled strain rate mode and controlled stress mode. Extensional flow is difficult to measure reliably in Laboratory circumstances. In this thesis we first present an updated control scheme that allows us to control the kinematics of polymer melts in an FSR, which is the foundation of our experimental work. Next we investigate four categories of polymer melts from the simplest system to the most complicated system, including 1) the narrow molar mass distribution (NMMD) linear polystyrene melts and solutions; 2) the bidisperse and polydisperse linear polystyrene melts; 3) the NMMD branched polystyrene melts; and 4) the polydisperse branched polylethylene melts. The experimental results are also compared with some developing theoretical models. Finally, to ensure the experimental data is accurate, the measurements from the FSR are compared with the data from some other extensional rheometers as well.

**General information**

State: Published
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**MPC for Wind Power Gradients - Utilizing Forecasts, Rotor Inertia, and Central Energy Storage**

We consider the control of a wind power plant, possibly consisting of many individual wind turbines. The goal is to maximize the energy delivered to the power grid under very strict grid requirements to power quality. We define an extremely low power output gradient and demonstrate how decentralized energy storage in the turbines' inertia combined with a central storage unit or deferrable consumers can be utilized to achieve this goal at a minimum cost. We propose a variation on model predictive control to incorporate predictions of wind speed. Due to the aerodynamics of the turbines the model contains nonconvex terms. To handle this nonconvexity, we propose a sequential convex optimization method, which typically converges in fewer than 10 iterations. We demonstrate our method in simulations with various wind scenarios and prices for energy storage. These simulations show substantial improvements in terms of limiting the power ramp rates (disturbance rejection) at the cost of very little power. This capability is critical to help balance and stabilize the future power grid with a large penetration of intermittent renewable energy sources.

**General information**

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**Multiple Scenario Generation of Subsurface Models: Consistent Integration of Information from Geophysical and Geological Data through Combination of Probabilistic Inverse Problem Theory and Geostatistics**
In geosciences, as well as in astrophysics, direct observations of a studied physical system and objects are not always accessible. Instead, indirect observations have to be used in order to obtain information about the unknown system, which leads to an inverse problem. Such geoscientific inverse problems face the challenge of determining a set of unknown model parameters based on a set of indirect observations of the subsurface. In a traditional least-squares formulation of the solution to an inverse problem, a subjectively chosen regularization parameter is used to obtain a unique solution to this problem, which leads to a smooth solution with no geological realism. Moreover, such a optimization-based framework does not allow introducing realistic geological prior information (due to a vectorial normed space structure). This thesis focuses on a more sophisticated approach based on a probabilistic formulation of the solution to the inverse problem. In this formulation, different sources of information about the subsurface can be weighted with regard to their relative quality and reliability (i.e., uncertainties) using probability distributions and subsequently integrated into a posterior probability distribution over the model parameters. The different sources of information are provided in form of a set of observed data, uncertainties related to the data, and geological prior information, which is established from, e.g., expert knowledge and old data sets. The prior information, when being informative and realistic, has a regulating effect on the solution to the inverse problem as geological and geophysical information are orthogonal in some ways, which allows reducing the underdetermination of the inverse problem. At the same time, such prior information also reduces the effective dimension of the inverse problem, which may considerably reduce the computationally cost related to such problems. Moreover, the probabilistic formulation of the inverse problem allows the use of geologically more realistic prior information that leads to solutions to the inverse problem with a higher degree of geological realism. Finally, the probabilistic formulation provides a means of analyzing uncertainties and potential multiple-scenario solutions to be used for risk assessments in relation to, e.g., reservoir characterization and forecasting. Prior models rely on information from old data sets or expert knowledge in form of, e.g., training images that expresses structural, lithological, or textural features. Statistics obtained from these types of observations will be referred to as sample models. Geostatistical sampling algorithms use a sample model as input and produce multiple realizations of the model parameters that, to some degree, honor this information. Such algorithms can be used to define the prior information for probabilistic inverse problems. In this way, very informative and geologically more realistic prior information can be provided. This thesis provides an overview of the scientific developments within the fields of probabilistic inverse problem theory and geostatistics, with emphasis on the combination of these scientific disciplines. In particular, the focus will be on consistent probabilistic formulations of this problem, which means that a correct weighting of the different sources of information is obeyed such that no unknown assumptions and biases influence the solution to the inverse problem. This involves a definition of the probabilistically formulated inverse problem, a discussion about how prior models can be established based on statistical information from sample models, and an analysis of geostatistical algorithms in order to understand the implicit assumptions made by such “black box” algorithms. A description of the posterior distribution can be obtained by drawing a representative sample from this distribution. Methodologies to be used for this purpose are presented. An example of sampling the posterior probability distribution of a computationally hard full waveform inverse problem using prior information based on multiple-point statistics, obtained from a training image, is demonstrated. For some computationally challenging inverse problems, a sample from the posterior distribution might still be too laborious to be obtained. Instead, a set of model parameters with (near) maximum posterior probability can be obtained. In order to do this, a closed form mathematical formulation of the prior probability distribution has to be established, such that the posterior probability distribution can be evaluated. Different solutions to this problem are presented and discussed. The prior probability distribution that is sampled by geostatistical sampling algorithms is typically unknown or sometime only a part of or an approximation to the distribution is known. This thesis provides an analysis and a discussion of how these prior probability distributions can be established, such that it is consistent with information provided by a known sample model. It is described how assumptions about the distribution, in addition to the information provided by the sample model, have to be made in order to end up with a unique solution to this problem. It is shown that these sampling algorithms typically provide samples from a prior probability distribution that is not consistent with the sample model. However, examples of consistent algorithms are also provided. A likelihood function is part of the probabilistic formulation of the inverse problem. This function is based on an uncertainty model that describes the uncertainties related to the observed data. In a similar way, a formulation of the prior probability distribution that takes into account uncertainties related to the sample model statistics is formulated. Prior models that are consistent with the statistics from a training image do not necessarily produce realizations with the same spatial patterns as seen in the training image because the local Markov properties that is satisfied in this way does not lead to a global reproduction of the pattern distribution from the training image. A prior probability distribution, with realizations that resemble the patterns as seen in the training image, is described and an efficient sampling algorithm that samples this distribution is provided. Moreover, an example of using this prior model for an inverse problem is demonstrated. The theoretical forward problem that describes the relation between data and model parameters is often associated with some degree of approximation. This approximation may have a great impact on the solution to the inverse problem because such approximate calculations of the data have an impact similar to observation uncertainties. We refer to the effect of these approximations as modeling errors. Examples that show how the modeling error is estimated are provided. Moreover, it is shown how these effects can be taken into account in the formulation of the posterior probability distribution. Common to the methods and strategies presented in this thesis is that they strive for a solution to the inverse problem that is consistent with the available information and to a less degree based on unconscious or subjective choices and implicit assumptions. Future studies related to theoretical developments of these strategies have to be provided. Moreover, applications of these strategies will reveal the practical implications of these consistent formulations. This will in particular be of great importance when it comes to assessments related cases of high risk such as human health or resources of high economical potentials.
Nonconvex Model Predictive Control for Commercial Refrigeration

We consider the control of a commercial multi-zone refrigeration system, consisting of several cooling units that share a common compressor, and is used to cool multiple areas or rooms. In each time period we choose cooling capacity to each unit and a common evaporation temperature. The goal is to minimize the total energy cost, using real-time electricity prices, while obeying temperature constraints on the zones. We propose a variation on model predictive control to achieve this goal. When the right variables are used, the dynamics of the system are linear, and the constraints are convex. The cost function, however, is nonconvex due to the temperature dependence of thermodynamic efficiency. To handle this nonconvexity we propose a sequential convex optimization method, which typically converges in fewer than 5 or so iterations. We employ a fast convex quadratic programming solver to carry out the iterations, which is more than fast enough to run in real-time. We demonstrate our method on a realistic model, with a full year simulation and 15 minute time periods, using historical electricity prices and weather data, as well as random variations in thermal load. These simulations show substantial cost savings, on the order of 30%, compared to a standard thermostat-based control system. Perhaps more important, we see that the method exhibits sophisticated response to real-time variations in electricity prices. This demand response is critical to help balance real-time uncertainties in generation capacity associated with large penetration of intermittent renewable energy sources in a future smart grid.
Nonlinear Model Predictive Control for Oil Reservoirs Management

The current world average recovery factor from oil fields is widely agreed to be about 30-35%. An increase of 10% point of this recovery factor would bring about 500 billion of oil barrels, sufficient to meet 16 years of current global production. To realize this potential production increase, the research community is working on improving current feedback model-based optimal control technologies. The topic of this thesis is production optimization for water flooding in the secondary phase of oil recovery. We developed numerical methods for nonlinear model predictive control (NMPC) of an oil field. The controller consists of

- A model based optimizer for maximizing some predicted financial measure of the reservoir (e.g. the net present value).
- A parameter and state estimator.
- Use of the moving horizon principle for data assimilation and implementation of the computed control input.

The optimizer uses gradient-based optimization and the required gradients are computed by the adjoint method. We propose the use of efficient high order implicit time integration methods for the solution of the forward and the adjoint equations of the dynamical model. The Ensemble Kalman filter is used for data assimilation. Further, we studied the use of robust control strategies in both open-loop, i.e. without measurement feedback, and closed-loop, i.e. with measurement feedback, configurations.

This thesis has three main original contributions:

The first contribution in this thesis is to improve the computationally expensive gradient computation by using high-order ESDIRK (Explicit Singly Diagonally Implicit Runge-Kutta) temporal integration methods and continuous adjoints. The high order integration scheme allows larger time steps and therefore faster solution times. We compare gradient computation by the continuous adjoint method to the discrete adjoint method and the finite-difference method. We demonstrate that the optimization algorithm can be accelerated by using the continuous time adjoint equations. This is the first time in the literature that the higher order continuous adjoint and higher order discrete adjoint methods have been investigated for oil production optimization.

The second contribution of this thesis is the application of the Robust Optimization strategy in both open-loop (i.e. without measurement feedback) and closed-loop (i.e. with measurement feedback). In the oil industry, Robust Optimization has been suggested to compensate for inherent geological uncertainties in an oil field. In robust optimization of an oil reservoir, the water injection and production borehole pressures are computed such that the predicted net present value of an ensemble of permeability field realizations is maximized. In our study, the permeability field is the uncertain parameters. We compare the performance of the RO strategy to a certainty equivalent optimization strategy, based on the ensemble mean of the permeability field realizations as its permeability field, and to a reactive strategy. In open-loop, for the case studied, the reactive strategy performed better than the open-loop RO strategy. These observations are nontrivial, as previous literature suggests that the open-loop RO strategy performs better than the reactive strategy. Simulations indicate that the inferior performance of the open-loop RO strategy compared to the reactive strategy is due to the inability of the RO strategy to efficiently encompass ensembles with very different and conflicting optimal control trajectories. Hence, we propose a modified RO strategy that allow shut in of uneconomical wells. The modified RO strategy performs significantly better than the other open-loop strategies and the reactive strategy. Finally, this is the first time in literature that the RO optimization has been investigated in closed-loop. Surprisingly, for the case studied, the closedloop certainty equivalent strategy yields a higher NPV than the closed-loop RO strategy. The uncertainty reduction of the permeability field estimate due to data assimilation explains the good performance of the closed-loop certainty equivalent optimization strategy. Consequently, in closed-loop, the increased computational effort of the RO strategy compared to the certainty equivalent strategy is not justified for the particular case studied in this paper.

The third contribution of this thesis is a mean-variance method for risk mitigation in production optimization of oil reservoirs. We introduce a return-risk bicriterion objective function for the profit-risk tradeoff. With this objective function we link the optimization problem in production optimization to the Markowitz portfolio optimization problem in finance or to the robust design problem in topology optimization. In this study we focus on open-loop configuration, i.e. without measurement feedback. We demonstrate that a return-risk bi-criterion objective function is a valuable tool for the profit-risk tradeoff. If combined with the previous contribution, this result trigger the necessity of comparing the closed-loop CE strategy with the closed-loop MV strategy.

The thesis consists of a summary report and a collection of five research papers written during the period May 2010 to August 2013. Three papers are published in conference proceedings, one paper is published in Computational Geosciences journal and another paper is submitted to Journal of Petroleum Science and Engineering.

General information
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Novel cross-linkers for PDMS networks for controlled and well distributed grafting of functionalities by click chemistry

An azide-containing, trifunctional vinyl cross-linker for silicone networks has been synthesized. The cross-linker has through Cu(i) catalyzed 1,3-cycloaddition been reacted with six different alkyne-containing chemical groups which each possess a particular functionality. The functional cross-linkers have been utilized to prepare novel polydimethylsiloxane (PDMS) networks. All functional cross-linkers were successfully incorporated into the networks and were demonstrated to be well distributed within the PDMS films. This was substantiated by fluorescence microscopy of a film prepared with the 4-methyl-umbelliferone containing cross-linker. TGA showed that a ferrocene functionality increased the thermal degradation temperature of PDMS. It was furthermore shown that the incorporation of only 0.25 wt% of the push-pull dipole, ethynyl-4-nitrobenzene, increased the dielectric permittivity of PDMS by 35%. The contact angle of PDMS films was increased from 108° to 116° by the introduction of a small poly(pentafluorostyrene) chain. Finally, 17α-ethynyl-1,3,5(10)-estratriene-3,17β-diol and 1-ethynyl-3,5- bis(trifluoromethyl)benzene were incorporated as examples of other functional groups. © 2013 The Royal Society of Chemistry.
Novel silicone compatible cross-linkers for controlled functionalization of PDMS networks

Polydimethylsiloxane (PDMS) elastomers are excellent materials for dielectric electroactive polymers (DEAPs) due to their high efficiency and fast response. PDMS suffers, however, from low dielectric permittivity and high voltages are therefore required when the material is used for DEAP actuators. In order to improve the dielectric properties of PDMS a novel system is developed where push-pull dipoles are grafted to a new silicone compatible cross-linker. The grafted cross-linkers are prepared by reaction of two different push-pull dipole alkynes as well as a fluorescent alkyne with the new azide-functional cross-linker by click chemistry. The dipole cross-linkers are used to prepare PDMS elastomers of various chain lengths providing different network densities. The functionalized cross-linkers are incorporated successfully into the networks and are well distributed as determined by the fluorescent functional cross-linker and fluorescence microscopy. The thermal, mechanical and electro-mechanical properties of PDMS elastomers of 0 wt% to 3.6 wt% of push-pull dipole cross-linker are investigated. An increase in the dielectric permittivity of 19% at only 0.46 wt% of pure push-pull dipole is observed. Furthermore, the dielectric losses are found to be very low while the electrical breakdown strengths are high and adequate for DEAP applications. © 2013 SPIE.

Novel silicone elastomer formulations for DEAPs

We demonstrate that the force output and work density of polydimethylsiloxane (PDMS) based dielectric elastomer transducers can be significantly enhanced by the addition of high permittivity titanium dioxide nanoparticles which was also shown by Stoyanov et al[1] for pre-stretched elastomers and by Carpi et al for RTV silicones[2]. Furthermore the elastomer matrix is optimized to give very high breakdown strengths. We obtain an increase in the dielectric permittivity of...
a factor of approximately 2 with a loading of 12% TiO2 particles compared to the pure modified silicone elastomer with breakdown strengths remaining more or less unaffected by the loading of TiO2 particles. Breakdown strengths were measured in the range from approximately 80-150 V/μm with averages of the order of 120-130 V/μm for the modified silicone elastomer with loadings ranging from 0 to 12%.

**General information**

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**Nuclear Magnetic Resonance and Elastic Wave Velocity of Chalk Saturated with Brines Containing Divalent Ions**

Nuclear magnetic resonance (NMR) has proven a good technique for measuring pore size distribution in reservoir rocks. The use of low field NMR together with sonic and electrical resistivity measurements, can contribute to illustrate the effect of adsorbing ions on chalk elasticity. NMR is useful for the study of the physical and chemical phenomena within saturated cores and sonic velocity is intimately connected to density and elastic constants of the rock. In this study we relate NMR data to changes in P-wave velocity due to ion adsorption. Core plugs from outcrop Stevns chalk, of ~45% porosity, were divided into groups of three and each group was saturated either with deionized water, calcite equilibrated water, or sodium chloride, magnesium chloride and calcium chloride solutions of the same ionic strength. Saturation with solutions that contain divalent ions caused major shifts in the distribution of the relaxation time. Core samples saturated with calcium chloride solution relaxed slower and those saturated with magnesium chloride solution relaxed faster than the rest of the samples. Along with the changes in relaxation the samples experienced smaller velocities of elastic waves when saturated with MgCl2 solution. Rock samples saturated with brines containing salts experienced lower electrical resistivity.

**General information**

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**Nuclear magnetic resonance and sound velocity measurements of chalk saturated with magnesium rich brine**

The use of low field Nuclear Magnetic Resonance (NMR) to determine petrophysical properties of reservoirs has proved to be a good technique. Together with sonic and electrical resistivity measurements, NMR can contribute to illustrate the changes on chalk elasticity due to different pore water composition. In this study we relate NMR data to changes in P-wave velocity and electrical resistivity. Core plugs from outcrop Stevns chalk, of 44% porosity, were divided into groups of three and saturated with deionized water, calcite equilibrated water, as well as sodium chloride and magnesium chloride solutions of the same ionic strength. Saturation with a solution that contained divalent ions caused major shifts in the distribution of the relaxation time. The changes were probably due to precipitates forming extra internal surface in the sample. Sonic velocities were relatively low in the MgCl2 solution saturated plugs.
Numerical analysis of a one-dimensional multicompontent model of the in-situ combustion process

An advanced numerical model for the in-situ combustion process is developed and studied in detail. The model is based on further extension and modification of the virtual kinetic cell (VKC) and virtual combustion tube (VCT) developed by Kristensen et al. (2007) and Kristensen (2008). Moreover, the model is based on SARA representation of a petroleum mixture (saturates–aromatics–resins–asphaltenes), which may react differently with oxygen and produce other components (for example, light oils and coke). In total, the model contains 14 components, which may undergo 15 chemical reactions. The set of reactions in the original model of M.R. Kristensen has been modified in order to account for secondary combustion of the light oil fraction. The results of the model implementation are applied to the four heavy oil systems and qualitatively compared to the results of previous experimental studies. A new parameter, the critical ignition saturation, is introduced, in order to describe the easiness of oil ignition. Its dependence on the different parameters of the oil mixture and injection gas is studied. The conclusions on the processes governing the ignition of oil in the presence of water are made. A parameter which affects most the possibility of ignition is the activation energy of the light fraction of the oil.
Online measurement of mass density and viscosity of pL fluid samples with suspended microchannel resonator

Physical characterization of viscous samples is crucial in chemical, pharma and petroleum industry. For example, in the refining industry of petroleum, water percentage is verified by measuring the density of a sample. In this article we present a suspended microchannel resonator (SMR) which uses 5 pL of a fluid sample and measures its density with a resolution of 0.01 kg/m$^3$ and a sensitivity of 16 Hz/kg/m$^3$. The resonator can also simultaneously measure viscosity of the solutions with an accuracy of 0.025 mPa s. The SMR is part of a system which contains packaging and tubing to deliver samples to the resonator. The system can easily handle multiple viscous fluids to measure their densities and viscosities. The SMR is transparent, facilitating visual inspection of the microchannel content. © 2013 Elsevier B.V.
Parallel Implementation of Riccati Recursion for Solving Linear-Quadratic Control Problems

In both Active-Set (AS) and Interior-Point (IP) algorithms for Model Predictive Control (MPC), sub-problems in the form of linear-quadratic (LQ) control problems need to be solved at each iteration. The solution of these sub-problems is usually the main computational effort. In this paper an alternative version of the Riccati recursion solver for LQ control problems is presented. The performance of both the classical and the alternative version is analyzed from a theoretical as well as a numerical point of view, and the alternative version is found to be approximately 50% faster than the classical one, for systems with many states. A number of parallel implementations of the alternative version has been proposed and tested.

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Petrophysical Analysis of Siliceous Ooze Sediments, Ormen Lange Field, Norway

Skeletal remains of siliceous algae form biogenic fine grained highly porous pelagic siliceous ooze sediments that were found above the reservoir of the Ormen Lange gas field which is located in the southern part of the Norwegian Sea (Figure 1a). The Palaeocene sandstone of the “Egga” Formation is the main gas reservoir (NDP). In this study, we are interested in the siliceous ooze intervals only.

A possible hydrocarbon prospect of siliceous ooze is proposed, but siliceous ooze is significantly different in structure from most commonly known hydrocarbon reservoir rocks. For instance, the pore structure is complex and the solids are mechanically fragile and hydrous. Normal petrophysical methods used in formation evaluation might not be suitable for interpreting siliceous ooze. For example, density and neutron logging tools are calibrated to give correct porosity readings in a limestone formation, but apparent porosity indications in any other lithology, such as siliceous ooze, are wrong and they should be corrected. The apparent bulk density log should be influenced by the hydrogen in opal as also the neutron porosity tools because they are sensitive to the amount of hydrogen in a formation and to a lesser extent upon other elements. It is normally assumed that the contribution to the neutron porosity measurement comes entirely from the hydrogen in fluids fully occupying the pore space. But, elements other than hydrogen that exist in the rock matrix do contribute to the signal; and hydrogen is also present in the solid. Some minerals of siliceous ooze, such as opal, have hydrogen in their structures which influences the measured hydrogen index (HI). The neutron tool obtains the combined signal of the HI of the solid phase and of the water that occupies the true porosity. The HI is equal to true porosity for completely freshwater saturated limestone. In this study, all the possible contributions to the neutron porosity measurement have been considered. Therefore, the slowing down power of all siliceous ooze minerals is taken into account.

In this study we aimed to develop and use a new procedure to analyse and interpret logging data acquired through siliceous ooze sediments. Our main objectives were to characterize and evaluate the petrophysics of siliceous ooze and to find the true porosity and water saturation to test its hydrocarbon reservoir potential. We used and integrated core analysis data with logging data from four Ormen Lange wells, and included X-ray diffraction analysis (XRD) data. Additionally, other available information such as petrographic thin-section analysis, core computed tomography scans (CT-scans), scanning electron microscope (SEM), and other published data were used here to interpret lithology and the unusual physical properties of the studied intervals. The integration of all these data revealed that the studied siliceous ooze is a mixture of opal and non-opal (shale). Our results proved to be reasonably consistent. The studied intervals apparently do not contain hydrocarbons.
Poroelasticity of high porosity chalk under depletion

The theory of poroelasticity for the elastic region below pore collapse by means of three different loading paths gives the possibility to compare the static and dynamically determined Biot coefficient for a set of experimental data with uniaxial loading on outcrop chalk performed with different levels of pore pressure. The chalk is oil-saturated Lixhe chalk from a quarry near Liège, Belgium, with a general porosity of 45%. Additionally, we compare the theoretical lateral stress to the experimentally determined lateral stress at the onset of pore collapse.

The static Biot coefficient based on mechanical test results is found to be lower than the pretest dynamic Biot coefficient determined from elastic wave propagation for the loading path and with less deviation under depletion. The calculated lateral stress is lower than the experimentally measured lateral stress depending on loading path. An explanation to this behaviour is pore pressure build up.

Potential theory of adsorption for associating mixtures: possibilities and limitations

The applicability of the Multicomponent Potential Theory of Adsorption (MPTA) for prediction of the adsorption equilibrium of several associating binary mixtures on different industrial adsorbents is investigated. In the MPTA the adsorbates are considered to be distributed fluids subject to an external potential field emitted by the adsorbent. In this work, the theory is extended to include the Cubic-Plus-Association (CPA) equation of state (EoS), for the description of the fluid-fluid interactions of associating mixtures. The Dubinin-Radushkevich-Astakhov (DRA) potential function is utilized to describe the solid-fluid interactions. The potential is extended to include adsorbate-absorbent specific capacities rather than an adsorbent specific capacity. Correlations of pure component isotherms are generally excellent with individual capacities, although adsorption on silicas at different temperatures still poses a challenge. The quality of the correlations is usually independent on the applied EoS. Predictions for binary mixtures indicate that the MPTA+SRK is superior when adsorption occurs on non-polar or slightly polar adsorbents, while MPTA+CPA performs better for polar adsorbents, or when the binary mixtures only contain associating compounds. Predictions are typically improved by about 3% when individual capacities and the best performing EoS are used, average absolute deviations of the selectivity are as low as 7-12%. Predictions of the selectivity are generally superior to predictions of the adsorbed amounts. The sensitivity of the model has also been tested, and it is concluded, that predictions are very sensitive to the adsorption energies.
In this thesis, we consider the control of two different industrial applications that belong at either end of the electricity grid; a power consumer in the form of a commercial refrigeration system, and wind turbines for power production. Our primary studies deal with economic model predictive control of a commercial multi-zone refrigeration system, consisting of several cooling units that share a common compressor, and is used to cool multiple areas or rooms, e.g., in supermarkets.

Substantial amounts of energy are consumed in refrigeration systems worldwide and there is a strong motivation for introducing more energy efficient as well as cost reducing control techniques. At the same time, the power grid is evolving from a centralized system with rather controllable production in the conventional power plants to a much more decentralized network of many independent power generators and a large penetration of renewable, fossil-free energy sources such as solar and wind power. To facilitate such intermittent producers, we must not only control the production of electricity, but also the consumption, in an efficient and exible manner. By enabling the use of thermal energy storage in supermarkets, we open up for exible power consumption schemes with the possibility of reducing operational costs and we develop and demonstrate prototype control technology that creates completely new business opportunities for selling regulating power to the grid. Moreover, this enables a larger penetration of wind energy in the power production and increases the potential market size for wind power generators and other renewable energy sources. Thus, we aim at promoting the use of environmentally sustainable power production technologies while creating new business opportunities for both power consumers and producers of renewable energy.

The second application, wind turbines, takes us to the production side of the power grid. The key concern here is to improve the quality and integrability of power delivered to the grid from large parks of wind turbines. Our goal is to reduce the fluctuating nature of the power output and to meet tightened demands from the grid by enabling a more intelligent control at both the individual turbine level, at the park controller level, and in cooperation with exible power consumers or other means of energy storage. The possible interaction and synergies of the two applications are obvious reasons to consider both in this thesis, and as we will see, the similarities in our formulations of the different control problems allow us to apply almost identical techniques despite the lack of immediate similarity.

For control of the commercial refrigeration application as well as the wind turbine application, we propose an economic optimizing model predictive controller, economic MPC. MPC is a feedback control technique that is characterized by its explicit handling of constrained control problems in which a model is used to predict the future behavior of a system along with forecasts of future disturbances. At each time step the values of the control inputs are computed by solving an open-loop finite time optimal control problem over a defined prediction horizon. Only the first step in this optimal open-loop sequence is implemented as a control command. Feedback is obtained by solving the open-loop problem repeatedly, in a receding horizon fashion, as new predictions become available.

Our investigations are primarily concerned with: 1) modeling of the applications to suit the chosen control framework; 2) formulating the MPC controller laws to overcome challenges introduced by the industrial applications, and defining economic objectives that reect the real physics of the systems as well as our control objectives; 3) solving the involved, non-trivial optimization problems efficiently in real-time; 4) demonstrating the feasibility and potential of the proposed methods by extensive simulation and comparison with existing control methods and evaluation of data from systems in actual operation.

We present contributions on:
-Linear economic MPC formulations that utilize the exibility in refrigeration systems to counteract fluctuations in the balance between power consumption and production.
-Economic MPC with probabilistic constraints, ensuring a robust performance and constraint satisfaction in spite of inaccurate system models and forecasts.
-Nonlinear economic MPC, reecting the nonconvexity in the realistic description of temperature dependent efficiencies in the refrigeration cycle.
-Nonlinear economic MPC with uncertain predictions and the implementation of very simple predictors that use entirely historical data of, e.g., electricity prices and outdoor temperatures.
Economic MPC for wind turbines, including
- Optimal steady-state calculation for wind farms.
- Nonlinear economic MPC for individual turbines.
- Change of variables and convex formulations of economic MPC for individual turbines.

Tractable optimization methods for the MPC problems, including
- Sequential convex programming (SCP) for specific nonconvex problems originating from our studies of commercial refrigeration as well as from our studies concerning wind power.
- Successful demonstration of the SCP approach on three different problems the commercial refrigeration system with linear dynamics and constraints and a nonconvex objective, the individual wind turbine with nonlinear dynamics and constraints, and the static optimization of the wind farm with a black-box model.

The major contribution is the formulation of these problems and the demonstrations to show that the SCP method can be used for their solution.

We demonstrate, i.a., substantial cost savings, on the order of 30 %, compared to a standard thermostat-based supermarket refrigeration system and show how our methods exhibit sophisticated demand response to real-time variations in electricity prices. Violations of the temperature ranges can be kept at a very low frequency of occurrence inspite of the presence of uncertainty. For the power output from wind turbines, ramp rates, as low a 3 % of the rated power per minute, can be effectively ensured with the use of energy storage and we show how the active use of rotor inertia as an additional energy storage can reduce the needed storage capacity by up to 30 % without reducing the power output.

General information
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Practical Implementations of Advanced Process Control for Linear Systems
Most advanced process control systems are based on Model Predictive Control (MPC). In this paper we discuss three critical issues for the practical implementation of linear MPC for process control applications. The rst issue is related to oset free control and disturbance models; the second issue is related to the use of soft output constraints in MPC; and the third issue is related to the computationally ecient solution of the quadratic program in the dynamic regulator of the MPC.
We have implemented MPC in .Net using C# and the MPCMath library. The implemented MPC is based on the target-regulator structure.
It enables oset free control; it can be computed eciently on-line using several optimization algorithms; and accommodates soft constraint for the outputs and for shaping the set-point tracking penalty function. We report selected observations using this implementation and discuss their practical implications for process control. If the control and evaluation intervals are chosen too short, the predicted behaviour of the controllers may have unstable characteristics. Depending of the degrees of freedom, oset-free control of a number of the controlled variables can be achieved by introduction of noise models and integration of the innovation errors. If the disturbances increases, oset-free control cannot be achieved without violation of process constraints. A target calculation function is used to calculate the optimal achievable target for the process. The use of soft constraints for process output constraints in the MPC controllers, ensures feasible solutions. The computational load as function of controllers type, model dimension and constraint type are shown.

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Prediction of Surfactant-related Properties for Chemical-based Product Design

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Prediction of thermo-physical properties of liquid formulated products
The objective of this chapter is to give an overview of the models, methods and tools that may be used for the estimation of liquid formulated products. First a classification of the products is given and the thermo-physical properties needed to represent their functions are listed. For each property, a collection of the available models are presented according to the property type and the model type. It should be noted, however, that the property models considered or highlighted in this chapter are only examples and are not necessarily the best and most accurate for the corresponding property.

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Organisations: Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, CERE – Center for Energy Ressources Engineering
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Prediction of the vapor–liquid equilibria and speed of sound in binary systems of 1-alkanols and n-alkanes with the simplified PC-SAFT equation of state
Prediction of speed of sound is a challenging task for any equation of state because it needs the first- and second-order derivatives of the Helmholtz free energy with respect to both temperature and volume. Equally challenging is the simultaneous predictions of phase behavior and speed of sound (or other derivative properties) with satisfactory accuracy over wide temperature, pressure and composition conditions. This work presents the prediction of the vapor–liquid equilibria and speed of sound in binary mixtures of 1-alkanols and n-alkanes using the simplified PC-SAFT equation of
state with pure component parameters estimated in different ways. All results are straight predictions, i.e. no binary
interaction parameters are used. With the parameters presented in this work, the predicted overall percent average
absolute deviations are, respectively, around 6.1% for the saturation pressure for 1533 experimental data points in the
temperature range from 273 to 493K, and 1.7% for the speed of sound for 2490 experimental data points at temperature
between 293 and 318K and pressure up to 120MPa. The results reveal that it is possible to simultaneously model the
vapor–liquid equilibria and speed of sound with a satisfactory accuracy for 1-alkanols and n-alkanes binary systems within
the PC-SAFT framework.

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ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.152 SNIP 1.286 CiteScore 2.31
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.034 SNIP 1.234 CiteScore 2.26
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 0.986 SNIP 1.317
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.133 SNIP 1.164
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.227 SNIP 1.09
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.031 SNIP 1.151
Compliant porosity in the form of cracks is known to cause significant attenuation and velocity dispersion through pore pressure gradients and consequent relaxation, dubbed squirt flow. Squirt flow from cracks vanish at high confining stress due to crack closing. Studies on clay bearing sandstones, however, show high attenuation and velocity dispersion remaining at high confining stress. Such dispersion is proposed to be caused by pressure gradients induced by compliant porosity within clay inclusions. By modeling the response of two extreme systems we quantify the possible effects of such clay-squirt flow on the bulk modulus of a clay bearing sandstone. The predicted magnitude of the clay-squirt effect on the bulk modulus is compared with experimental data. The clay-squirt effect is found to possibly account for a significant portion of the deviations from Gassmann fluid substitution in claybearing sandstones.

Quantifying the effect of squirt flow dispersion from compliant clay porosity in clay bearing sandstones
Compliant porosity in the form of cracks is known to cause significant attenuation and velocity dispersion through pore pressure gradients and consequent relaxation, dubbed squirt flow. Squirt flow from cracks vanish at high confining stress due to crack closing. Studies on clay bearing sandstones, however, show high attenuation and velocity dispersion remaining at high confining stress. Such dispersion is proposed to be caused by pressure gradients induced by compliant porosity within clay inclusions. By modeling the response of two extreme systems we quantify the possible effects of such clay-squirt flow on the bulk modulus of a clay bearing sandstone. The predicted magnitude of the clay-squirt effect on the bulk modulus is compared with experimental data. The clay-squirt effect is found to possibly account for a significant portion of the deviations from Gassmann fluid substitution in claybearing sandstones.

General information
State: Published
Organisations: Department of Civil Engineering, Section for Geotechnics and Geology, Center for Energy Resources Engineering
Authors: Sørensen, M. K. (Intern), Fabricius, I. L. (Intern)
Pages: 249-258
Publication date: 2013

Host publication information
Title of host publication: Poromechanics V : Proceedings of the Fifth Biot Conference on Poromechanics
Publisher: American Society of Civil Engineers
ISBN (Print): 978-0-7844-1299-2
Main Research Area: Technical/natural sciences
Wave dispersion, Clays, Porosity, Sandstone, Cracking
DOIs:
10.1061/9780784412992.029
Source: dtu
Source-ID: n::oai:DTIC-ART:inspec/426496561::34794
Publication: Research - peer-review › Book chapter – Annual report year: 2013

Rate and Predictors of the Conversion of Abstracts Presented at the Canadian Cardiovascular Congress Scientific Meetings to Full Peer-Reviewed Publications
The rate of conversion of abstracts presented at scientific meetings into peer-reviewed published manuscripts is an important metric for medical societies, because it facilitates translation of scientific knowledge into practice. We determined the rate and predictors of conversion of scientific abstracts presented at the Canadian Cardiovascular Congress (CCC) from 2006 to 2010 into peer-reviewed article publications within 2 years of their initial presentation. Using a previously validated computer algorithm, we searched the International Statistical Institute Web of Science to identify
A multivariable logistic regression was used to identify independent factors associated with successful publication. From 2006 to 2010, 3565 abstracts were presented at the CCC. Overall 24.1% of presented abstracts were published within 2 years of the conference. Mean impact factor for publications was 5.2 (range, 0.4-53.2). The type of presentation (for poster vs oral; odds ratio, 0.71; 95% confidence interval, 0.60-0.83; P <0.001) and category of presentation (P <0.001) were significantly associated with successful publication. Late breaking abstracts and those related to cancer and clinical sciences were more likely to be published, compared with prevention, vascular biology, and pediatrics. In conclusion, the publication rate at the CCC is only marginally lower than that reported for large international North American and European cardiology conferences (30.6%). Efforts should focus on several identified barriers to improve conversion of abstracts to full report publication.

General information
State: Published
Organisations: Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering, University of Toronto, Copenhagen University Hospital
Pages: 1520-1523
Publication date: 2013
Main Research Area: Technical/natural sciences

Publication information
Journal: Canadian Journal of Cardiology
Volume: 29
Issue number: 11
ISSN (Print): 0828-282x
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.46 SJR 1.427 SNIP 1.091
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.358 SNIP 0.993 CiteScore 2.3
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.56 SNIP 1.166 CiteScore 2.56
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.232 SNIP 1.266 CiteScore 2.6
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.22 SNIP 0.995 CiteScore 2.05
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.718 SNIP 0.746 CiteScore 1.39
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.538 SNIP 0.5
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.616 SNIP 0.594
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.614 SNIP 0.566
Scopus rating (2007): SJR 0.81 SNIP 0.731
Scopus rating (2006): SJR 0.672 SNIP 0.809
Scopus rating (2005): SJR 0.69 SNIP 0.703
Scopus rating (2004): SJR 0.526 SNIP 0.654
Scopus rating (2003): SJR 0.541 SNIP 0.712
Scopus rating (2002): SJR 0.472 SNIP 0.509
Reinforced poly(propylene oxide)- a very soft and extensible dielectric electroactive polymer

Poly(propylene oxide) (PPO), a novel soft elastomeric material, and its composites were investigated as a new dielectric electroactive polymer (EAP). The PPO networks were obtained from thiol-ene chemistry by photochemical crosslinking of \( \text{\textalpha}\text{-diallyl PPO with a tetra-functional thiol. The elastomer was reinforced with hexamethylenedisilazane treated fumed silica to improve the mechanical properties of PPO. The mechanical properties of PPO and composites thereof were investigated by shear rheology and stress–strain measurements. It was found that incorporation of silica particles improved the stability of the otherwise mechanically weak pure PPO network. Dielectric spectroscopy revealed high relative dielectric permittivity of PPO at 103 Hz of 5.6. The relative permittivity was decreased slightly upon addition of fillers, but remained higher than the commonly used acrylic EAP material VHB4910. The electromechanical actuation performance of both PPO and its composites showed properties as good as VHB4910 and a lower viscous loss.

General information

State: Published
Organisations: Department of Chemical and Biochemical Engineering, The Danish Polymer Centre, Center for Energy Resources Engineering, University of Pisa
Authors: Goswami, K. (Intern), Galantini, F. (Ekstern), Mazurek, P. S. (Intern), Daugaard, A. E. (Intern), Gallone, G. (Ekstern), Skov, A. L. (Intern)
Publication date: 2013
Main Research Area: Technical/natural sciences

Publication information

Journal: Smart Materials and Structures
Volume: 22
ISSN (Print): 0964-1726
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 0.976 SNIP 1.547 CiteScore 3.1
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.156 SNIP 1.698 CiteScore 3.03
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.254 SNIP 1.869 CiteScore 2.9
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.023 SNIP 1.915 CiteScore 2.61
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.016 SNIP 1.764 CiteScore 2.19
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.196 SNIP 1.972 CiteScore 2.53
Response to Letters Regarding Article, "Conversion of Cardiovascular Conference Abstracts to Publications"

General information
State: Published
Organisations: Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering, Duke University
Authors: Fosbøll, E. L. (Ekstern), Harrington, R. A. (Ekstern), Eapen, Z. (Ekstern), Peterson, E. D. (Ekstern), Fosbøl, P. L. (Intern)
Pages: E29-E29
Publication date: 2013
Main Research Area: Technical/natural sciences

Publication information
Journal: Circulation
ISSN (Print): 0009-7322
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 8.41
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 8.52
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 8.54
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 9.32
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 9.57
Silicone resembling poly (propylene glycol) interpenetrating networks based on no pre-stretch as basis for electrical actuators

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, The Danish Polymer Centre, Center for Energy Resources Engineering
Authors: Goswami, K. (Intern), Bahrt, F. (Intern), Daugaard, A. E. (Intern), Skov, A. L. (Intern)
Publication date: 2013

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Title of host publication: Proceedings of SPIE
Volume: 8687
Publisher: SPIE - International Society for Optical Engineering
Editor: Bar-Cohen, Y.
Article number: 86871Z
Main Research Area: Technical/natural sciences
Conference: Electroactive Polymer Actuators and Devices 2013, San Diego, California, United States, 11/03/2013 - 11/03/2013
Poly (propylene glycol), IPN, Actuator, Dielectric permittivity
DOIs:
10.1117/12.2010494
Source: dtu
Source-ID: u::7511
Publication: Research - peer-review › Article in proceedings – Annual report year: 2013

SIPPI: A Matlab toolbox for sampling the solution to inverse problems with complex prior information: Part 1—Methodology
From a probabilistic point-of-view, the solution to an inverse problem can be seen as a combination of independent states of information quantified by probability density functions. Typically, these states of information are provided by a set of observed data and some a priori information on the solution. The combined states of information (i.e. the solution to the inverse problem) is a probability density function typically referred to as the a posteriori probability density function. We present a generic toolbox for Matlab and Gnu Octave called SIPPI that implements a number of methods for solving such probabilistically formulated inverse problems by sampling the a posteriori probability density function. In order to describe the a priori probability density function, we consider both simple Gaussian models and more complex (and realistic) a priori models based on higher order statistics. These a priori models can be used with both linear and non-linear inverse problems. For linear inverse Gaussian problems we make use of least-squares and kriging-based methods to describe the a posteriori probability density function directly. For general non-linear (i.e. non-Gaussian) inverse problems, we make use of the extended Metropolis algorithm to sample the a posteriori probability density function. Together with the extended Metropolis algorithm, we use sequential Gibbs sampling that allow computationally efficient sampling of complex a priori models. The toolbox can be applied to any inverse problem as long as a way of solving the forward problem is provided. Here we demonstrate the methods and algorithms available in SIPPI. An application of SIPPI, to a tomographic cross borehole inverse problems, is presented in a second part of this paper.

General information
State: Published
Organisations: Center for Energy Resources Engineering, Department of Applied Mathematics and Computer Science, Scientific Computing, University of Copenhagen
SIPPI: A Matlab toolbox for sampling the solution to inverse problems with complex prior information: Part 2—Application to crosshole GPR tomography

We present an application of the SIPPI Matlab toolbox, to obtain a sample from the a posteriori probability density function for the classical tomographic inversion problem. We consider a number of different forward models, linear and non-linear, such as ray based forward models that rely on the high frequency approximation of the wave-equation and 'fat' ray based forward models relying on finite frequency theory. In order to sample the a posteriori probability density function we make use of both least squares based inversion, for linear Gaussian inverse problems, and the extended Metropolis sampler, for non-linear non-Gaussian inverse problems. To illustrate the applicability of the SIPPI toolbox to a tomographic field data set we use a cross-borehole traveltime data set from Arrenæs, Denmark. Both the computer code and the data are released in the public domain using open source and open data licenses. The code has been developed to facilitate inversion of 2D and 3D travel time tomographic data using a wide range of possible a priori models and choices of forward models.

General information
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Organisations: Center for Energy Resources Engineering, Department of Applied Mathematics and Computer Science, Scientific Computing, University of Copenhagen
Authors: Hansen, T. M. (Intern), Cordua, K. S. (Intern), Looms, M. C. (Ekstern), Mosegaard, K. (Intern)
Pages: 481-492
Publication date: 2013
Main Research Area: Technical/natural sciences

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Volume: 52
ISSN (Print): 0098-3004
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 1.083 SNIP 1.736 CiteScore 2.93
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.213 SNIP 1.678 CiteScore 2.67
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.103 SNIP 1.798 CiteScore 2.52
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.815 SNIP 1.628 CiteScore 2.06
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.897 SNIP 1.807 CiteScore 2.1
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.902 SNIP 1.712 CiteScore 2.02
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.995 SNIP 1.649
BFI (2009): BFI-level 1
Solar/electric heating systems for the future energy system

The project “Solar/electric heating systems in the future energy system” was carried out in the period 2008-2013. The project partners were DTU Byg, DTU Informatics (now DTU Compute), DMI, ENFOR A/S and COWI A/S. The companies Ajva ApS, Ohmatex ApS and Innogie ApS worked together with the project partners in two connected projects in order to develop solar/electric heating systems for laboratory tests. The project was financed by the Danish Agency for Science, Technology and Innovation under the Danish Council for Strategic Research in the program Sustainable Energy and Environment. The DSF number of the project is 2104-07-0021/09-063201/DSF. This report is the final report of the project.

The aim of the project is to elucidate how individual heating units for single family houses are best designed in order to fit into the future energy system. The units are based on solar energy, electrical heating elements/heat pump, advanced heat storage tanks and advanced control systems.

Heat is produced by solar collectors in sunny periods and by electrical heating elements/heat pump. The electrical heating elements/heat pump will be in operation in periods where the heat demand cannot be covered by solar energy. The aim is to use the auxiliary heating units when the electricity price is low, e.g. due to large electricity production by wind turbines.

The unit is equipped with an advanced control system where the control of the auxiliary heating is based on forecasts of the electricity price, the heat demand and the solar energy production. Consequently, the control is based on weather forecasts.

Three differently designed heating units are tested in a laboratory test facility. The systems are compared on the basis of:
- energy consumption for the auxiliary heating
- energy cost for the auxiliary heating
- net utilized solar energy

General information

State: Published
Organisations: Department of Civil Engineering, Section for Building Physics and Services, Department of Applied Mathematics and Computer Science , Dynamical Systems, Center for Energy Resources Engineering, Scientific Computing, Department of Electrical Engineering, Danish Meteorological Institute , COWI A/S, Innogie ApS
Number of pages: 617
Publication date: 2013
Solving inverse problems through a smooth formulation of multiple-point geostatistics

In oil and gas sector accurate reservoir description play a crucial role in problems associated with recovery of hydrocarbons, risk estimation and predicting reservoir performance. Knowledge on reservoir properties can be inferred from measurements typically made at the surface by solving corresponding inverse problems. However, noise in data, non-linear relationships and sparse observations impede creation of realistic reservoir models. Including complex a priori information on reservoir parameters facilitates the process of obtaining acceptable solutions. Such a priori knowledge may be inferred, for instance, from a conceptual geological model termed a training image. The main motivation for this study was the challenge posed by history matching, an inverse problem aimed at estimating rock properties from production data. We addressed two main difficulties of the history matching problem: existence of multiple, most often geologically unfeasible, solutions and high computational cost of the forward simulation. The developed methodology resulted in a new method for solving inverse problems with training-image based a priori information, when the computational time matters. Specifically, we have proposed a smooth formulation of training-image based priors, which was inspired by the Frequency Matching method developed by our group earlier. The proposed smooth generalization, that integrates data and multiple-point statistics in a probabilistic framework, allows us to find solution by use of gradient-based optimization. As the result, solutions to an inverse problem may be obtained efficiently by deterministic search. We have applied the proposed methodology to the problem of history matching. Both the smooth formulation and the Frequency Matching method find the solution by maximizing its posterior probability. This is achieved by introducing a closed form expression for the a priori probability density. We have defined an expression for the training-image based prior by applying the theory of multinomial distributions. Its combination with the likelihood function results in the closed form expression for defining relative posterior probabilities of the solutions. Finally, we applied the developed smooth formulation to the problem of seismic inversion. This thesis reviews the latest developments in the field of geoscientific inverse problems with a focus on the history matching problem. The work contains detailed explanation of our strategies including both theoretical motivation and practical aspects of implementation. Finally, it is complemented by six research papers submitted, reviewed and/or published in the period 2010 - 2013.

Speeding up compositional reservoir simulation through an efficient implementation of phase equilibrium calculation

Compositional reservoir simulations are widely used to simulate reservoir processes with strong compositional effects, such as gas injection. The equations of state (EoS) based phase equilibrium calculation is a time consuming part in this type of simulations. The phase equilibrium problem can be either decoupled from or coupled with the transport problem. In the former case, flash calculation is required, which consists of stability analysis and subsequent phase split calculation; in the latter case, no explicit phase split calculation is required but efficient stability analysis and optimized coding of the basic thermodynamic subroutines are still crucial to the overall speed. This work tries to provide a comprehensive strategy to increase the speed for compositional simulation. This strategy begins with the coding of the basic thermodynamic properties, including the derivatives of fugacities with respect to molar numbers. Then, in the algorithms for stability analysis and phase split calculation, successive substitution with acceleration and minimization-based second-order methods are combined to gain both robustness and efficiency. For compositional simulations, the results from previous simulation steps provide the possibility to skip stability analysis by the shadow region method in the single phase regions.
The approach was implemented in the general purpose research simulator (GPRS) developed by Stanford University. GPRS is a modular, state of the art reservoir simulation and its architecture makes the implementation and evaluation of new ideas and concepts easy. Tests on several 2-D and 3-D gas injection examples indicate that with an efficient implementation of the thermodynamic package and the conventional stability analysis algorithm, the speed can be increased by several folds. Application of the shadow region method to skip stability analysis can further cut the phase equilibrium calculation time. Copyright 2013, Society of Petroleum Engineers.

Stimuli-Adaptable Materials

The work presented in this Thesis deals with the development of a stimuli-adaptable polymer material based on the UV-induced dimerisation of cinnamic acid and its derivatives. It is in the nature of an adhesive to adhere very well to its substrate and therefore problems can arise upon removal of the adhesive. This is also known from skin adhesives where it is very undesirable to cause damage to the skin. The overall idea of this project was to resolve this problem by developing a material which could switch between an adhesive and a non-adhesive state. Switchable adhesion is known in the literature but the presented work has a new approach to the field by basing itself on the idea of developing a network into which a photo-active polymer is mixed and which function as an adhesive. Upon irradiation with UV-light for a short time a non-adhering inter-penetrating network material would be formed. Two simple models for the extent of reaction for the system are presented and show that the timescale for the reaction is minutes to hours. This was further investigated with IR-spectroscopy and UV-absorbance spectroscopy. UV-spectroscopy confirmed that a change in the material occurs upon irradiation with UV and that the reaction time is in the range of minutes. A number of polymer derivatives with cinnamic acid or cinnamylidene acetic acid were prepared and the material properties of these were studied before and after irradiation with UV-light. For the cinnamylidene acetic acid derivatised polymers a macroscopic change was observed upon dissolution of the irradiated compound. The irradiated polymers formed threads or fibres when exposed to water while the unexposed polymers dissolved as a hygroscopic powder. Cinnamic acid derivatised poly(ethylene glycol) (PEG) was studied in detail and three different polymers were derivatised, namely a 4-armed star PEG (Mn = 2000 g/mol), a short linear PEG (Mn = 1000 g/mol) and a long linear PEG (Mn = 4000 g/mol). The derivatised polymers were mixed to create three different photo-active materials and these were investigated with rheology before and after irradiation with UV-light for one hour. It was observed that the largest change occurred for the system consisting solely of the cinnamic acid derivatised 4-armed star PEG. The development of the material properties of this material was studied in details by exposing the compound to UV-radiation for up to 120 h and determining the rheological properties after the exposure. It was found that approx. 24 hours was needed to form a manageable film and that approx. 70 hours were needed to obtain stable rheological properties. The exposure times were larger than expected but it was assumed that this would be resolved by preparation of the inter-penetrating network materials. A number of inter-penetrating network materials where both the permanent Network as well as the switching segment was made up of PEG-polymers were prepared. It was found that for a material with relatively long chains in both permanent Network (Mn = 10000 g/mol) and switching segment (Mn = 15000 g/mol) no changes occurred upon exposure to UV-light. It is expected that this is because Mn of polymers is above the molecular entanglement weight. Inter-penetrating network materials with Mn = 4000 g/mol in the permanent network were prepared. Initially a linear photo-active PEG was mixed into the material. This material exhibited a decrease in the values for G and G after irradiation with UV-light for 30 minutes. The reason for the decrease in the two rheological parameters is unclear but the change encouraged further work with this type of systems. Two inter-penetrating network materials with the star-shaped cinnamic acid derivatised PEG as switching segment were prepared and irradiated with UV-light for 72 hours. The network with r = 0.75 in the permanent matrix proved the expectations by clearly showing a solvent effect when the photo-active polymer was introduced into the permanent network. In addition a significant increase of G and G was observed after 72 h of irradiation with UV-light proving the formation of a second network consisting of the photo-
active polymers. A network with \( r = 0.5 \) in the permanent matrix was also investigated but gave very different results due to the lower value for \( r \). The applied \( r \)-value is significantly closer to the critical \( r_c \)-value and thus resulted in problems with the film formation. The data showed that the secondary network dominates the rheological properties of this network. A material with shorter chains in the permanent network (\( Mn = 1000 \) g/mol) was also investigated but showed no change after irradiation with UV-light for 15 minutes. This is related to the stiffness of permanent matrix. First steps to creating an inter-penetrating network with two different polymers were taken by incorporating the cinnamic acid derivatised PEG-stars into a poly(propylene oxide) network. However exposure to UV-light did not result in any changes of the material properties. It was also tested if the photo-active PEG could be incorporated into a poly(dimethyl siloxane) network, but the addition of the photo-active PEG resulted in complete hindrance of the cross-linking of the poly(dimethyl siloxane). A number of problems were identified throughout the work, primarily concerning the mismatch between the expected exposure time needed to induce changes in the materials and the exposure time observed experimentally. This can partially be explained by mobility of the polymers and concentration of the photo-active cinnamic acid. Studies presented in the literature show that the position of the cinnamic acid groups is important for the dimerisation to occur. The nature of polymers makes encounters between end groups less likely and this affects the dimerisation. Furthermore, an NMR-study showed formation of the cis-isomer of cinnamic acid. The isomerisation of cinnamic acid only occurs if dimerisation is hindered. This underlines that the circumstances are not ideal for dimerisation.
previous tie-line in the same grid-block to determine whether the approximation should be made. Comparison between the shadow-region approach and the approximation approach, including TTL and TDBA, has been made with a slimtube simulator by which the simulation temperature and the simulation pressure are set constant. It is shown that TDBA can significantly improve the speed in the two-phase region. In contrast, TTL, even with a precalculated tie-line table, is not so advantageous compared with an efficient implementation of rigorous flash. Furthermore, we implemented TDBA in a compositional streamline simulator to apply TDBA to scenarios with pressure variation across the reservoir. We also discussed how to extend TDBA to the general situation in which pressures in grid-blocks are updated dynamically.

**General information**

State: Published
Organisations: Department of Chemistry, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering, Center for Energy Resources Engineering, Technical University of Denmark
Authors: Yan, W. (Intern), Belkadi, A. (Intern), Michelsen, M. L. (Intern), Stenby, E. H. (Intern)
Pages: 932-942
Publication date: 2013
Main Research Area: Technical/natural sciences

**Publication information**

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Volume: 18
Issue number: 5
ISSN (Print): 1086-055X
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  - BFI (2018): BFI-level 1
  - Web of Science (2018): Indexed yes
  - BFI (2017): BFI-level 1
  - Web of Science (2017): Indexed Yes
  - BFI (2016): BFI-level 1
  - Scopus rating (2016): CiteScore 3.01 SJR 0.95 SNIP 2.003
  - Web of Science (2016): Indexed yes
  - BFI (2015): BFI-level 1
  - Scopus rating (2015): SJR 0.976 SNIP 1.838 CiteScore 2.37
  - BFI (2014): BFI-level 1
  - Scopus rating (2014): SJR 1.185 SNIP 2.152 CiteScore 2.43
  - BFI (2013): BFI-level 1
  - Scopus rating (2013): SJR 0.993 SNIP 1.773 CiteScore 2.25
  - ISI indexed (2013): ISI indexed yes
  - Web of Science (2013): Indexed yes
  - BFI (2012): BFI-level 1
  - Scopus rating (2012): SJR 1.047 SNIP 1.757 CiteScore 2.13
  - ISI indexed (2012): ISI indexed yes
  - BFI (2011): BFI-level 1
  - Scopus rating (2011): SJR 1.139 SNIP 1.757 CiteScore 2.3
  - ISI indexed (2011): ISI indexed yes
  - Web of Science (2011): Indexed yes
  - BFI (2010): BFI-level 1
  - Scopus rating (2010): SJR 1.143 SNIP 2.103
  - Web of Science (2010): Indexed yes
  - BFI (2009): BFI-level 1
  - Scopus rating (2009): SJR 1.106 SNIP 1.642
  - BFI (2008): BFI-level 1
  - Scopus rating (2008): SJR 0.513 SNIP 1.369
  - Scopus rating (2007): SJR 0.677 SNIP 0.894
  - Scopus rating (2006): SJR 1.09 SNIP 1.93
  - Web of Science (2006): Indexed yes
  - Scopus rating (2005): SJR 2.134 SNIP 1.808
  - Scopus rating (2004): SJR 2.536 SNIP 1.462
  - Scopus rating (2003): SJR 1.262 SNIP 0.922
Synergistic kinetic inhibition of natural gas hydrate formation

Rocking cells were used to investigate the natural gas hydrate formation and decomposition in the presence of kinetic inhibitor, Luvicap. In addition, the influence of poly ethylene oxide (PEO) and NaCl on the performance of Luvicap was investigated using temperature ramping and isothermal experiments. Luvicap decreased the hydrate nucleation temperature in ramping and increased the hydrate nucleation time at fixed temperatures. The presence of PEO and NaCl enhanced the nucleation inhibition strength of Luvicap. However the addition of Luvicap promoted the hydrate growth after nucleation. PEO does not affect hydrate growth whereas NaCl reduced the hydrate growth both in the presence and absence of Luvicap. In addition complex two-stage hydrate growth was observed in the presence of Luvicap. Moreover, the hydrate formed in the presence of inhibitor took longer time/higher temperature to decompose completely. One should consider this complex inhibitor-mediated hydrate formation and decomposition kinetics when screening and designing kinetic inhibitors for field applications.
**The Effect of Bacteria Penetration on Chalk Permeability**

Bacteria selective plugging is one of the mechanisms through which microorganisms can be applied for enhanced oil recovery. Bacteria can plug the water-bearing zones of a reservoir, thus altering the flow paths and improving sweep efficiency. It is known that the bacteria can penetrate deeply into reservoirs, however, a complete understanding of the penetration behavior of bacteria is lacking, especially in chalk formations where the pore throat sizes are almost comparable with the sizes of bacteria vegetative cells. This study investigates the penetration of bacteria into chalk. Two bacteria types, the spore forming Bacillus licheniformis 421 and the non-spore forming Pseudomonas putida K12, were used. The core plugs were Stevns Klint outcrop with initial permeability at 2-4 mD. The results revealed that bacteria were able to penetrate and to be transported through the chalk. Furthermore, a higher number of B. licheniformis was detected on the effluent compared with P. putida. However, in the experiment with B. licheniformis mainly spores were detected in the effluent. The core permeability decreased rapidly during injection of bacteria and a starvation period of 12 days did not allow the permeability to return to initial condition.

**General information**

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**Organisations:** Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering, Department of Systems Biology, Metabolic Signaling and Regulation  
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**Number of pages:** 4
The effect of kaolinite on the permeability

General information
State: Published
Organisations: Department of Civil Engineering, Section for Geotechnics and Geology, Center for Energy Resources Engineering, Geological Survey of Denmark and Greenland
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Publication: Research › Poster – Annual report year: 2013

The Homogeneous Interior-Point Algorithm: Nonsymmetric Cones, Warmstarting, and Applications

The overall topic of this thesis is convex conic optimization, a sub-field of mathematical optimization that attacks optimization problem with a certain geometric structure. These problems allow for modelling of an extremely wide range of real-world problems, but the availability of solution algorithms for these problems is still limited.

The goal of this thesis is to investigate and shed light on two computational aspects of homogeneous interior-point algorithms for convex conic optimization:
The first part studies the possibility of devising a homogeneous interior-point method aimed at solving problems involving constraints that require nonsymmetric cones in their formulation. The second part studies the possibility of warmstarting the homogeneous interior-point algorithm for conic problems. The main outcome of the first part is the introduction of a completely new homogeneous interior-point algorithm designed to solve nonsymmetric convex conic optimization problems. The algorithm is presented in detail and then analyzed. We prove its convergence and complexity. From a theoretical viewpoint, it is fully competitive with other algorithms and from a practical viewpoint, we show that it holds lots of potential, in several cases being superior to other solution methods.

The main outcome of the second part of the thesis is two new warmstarting schemes for the homogeneous interior-point algorithm for conic problems. Again, we first motivate and present the schemes and then analyze them. It is proved that they, under certain circumstances, result in an improved worst-case complexity as compared to a normal coldstart. We then move on to present an extensive series of computational results substantiating the practical usefulness of these warmstarting schemes. These experiments include standard benchmarking problem test sets as well as an application from smart energy systems.

General information
State: Published
Organisations: Department of Applied Mathematics and Computer Science, Scientific Computing, Center for Energy Resources Engineering
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Number of pages: 149
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Publisher: Technical University of Denmark (DTU)
Original language: English
The Potential of Economic Model Predictive Control for Spray Drying Plants

In 2015 the milk quota system in the European Union will be completely liberalized. As a result, analysts expect production of skimmed and whole milk powder to increase by 5-6% while its price will decline by about 6-7%. Multi-stage spray drying is the prime process for the production of food powders. The process is highly energy consuming and capacity depends among other factors on correct control of the dryer. Consequently efficient control and optimization of the spray drying process has become increasingly important to accommodate the future market challenges.

The goal of the presentation is to present our results regarding modeling of the process and how the efficiency and probability can be lifted by introducing an economic optimizing MPC scheme.

Firstly, we develop a first-principle engineering model that can be used to simulate spray drying processes with high accuracy. The model can be adjusted to describe drying of various products and describes the complete drying process of a multi-stage spray dryer. The dryer is divided into three stages, the spray stage and two uid bed stages. Each stage is assumed ideally mixed and described by mass- and energy balances. The model is able to predict outlet temperatures, the residual moisture and particle size of the product. We also give a novel approach to predict deposits due to stickiness of the powder. The model predictions are compared to datasets gathered at GEA Process Engineering's test facility. The identified model parameters are identified from data and the resulting model is the data well.

Secondly, the effect of disturbances, ambient air humidity and solids content in the feed, is studied by simulation. We show that conventional control is insufficient at controlling the product quality as well as driving the plant to the most economic conditions. Furthermore, we show that the efficiency can be increased by correct adjustment of heat and inlet air ow at each stage.

The recent focus in research has shifted from reference tracking MPC to optimization of economic objective functions. We will discuss how this optimization can be performed by advanced process control techniques, such as Economic Model Predictive Control (E-MPC). We suggest adding an E-MPC based supervisory control layer on top of the contemporary PI-controllers. The strong interconnection between drying stages and process onstraints are well suited for MPC.

General information
State: Published
Organisations: Department of Applied Mathematics and Computer Science , Scientific Computing, Dynamical Systems, Department of Electrical Engineering, Automation and Control, Center for Energy Resources Engineering, GEA Process Engineering A/S
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Number of pages: 1
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Thermal Storage Power Balancing with Model Predictive Control

The method described in this paper balances power production and consumption with a large number of thermal loads. Linear controllers are used for the loads to track a temperature set point, while Model Predictive Control (MPC) and model estimation of the load behavior are used for coordination. The total power consumption of all loads is controlled indirectly through a real-time price. The MPC incorporates forecasts of the power production and disturbances that influence the loads, e.g. time-varying weather forecasts, in order to react ahead of time. A simulation scenario demonstrates that the method allows for the integration of flexible thermal loads in a smart energy system in which consumption follows the changing production.
Thermodynamic Modeling of Natural Gas Systems Containing Water

As the need for dew point specifications remains very urgent in the natural gas industry, the development of accurate thermodynamic models, which will match experimental data and will allow reliable extrapolations, is needed. Accurate predictions of the gas phase water content in equilibrium with a heavy phase were previously obtained using cubic plus association (CPA) coupled with a solid phase model in the case of hydrates, for the binary systems of water–methane and water–nitrogen and a few natural gas mixtures. In this work, CPA is being validated against new experimental data, both water content and phase equilibrium data, and solid model parameters are being estimated for four natural gas main components (methane, ethane, propane, and carbon dioxide). Different tests for the solid model parameters are reported, including vapor-hydrate-equilibria (VHE) and liquid-hydrate-equilibria (LHE) calculations, structural transitions, and predictions at low temperatures. Furthermore, model predictions for representative multicomponent mixtures are presented and compared against the ISO-standard GERG-water model and other selected models. In most cases, very good agreement with experimental data is obtained.
Gas clathrate hydrate dissociation pressures are reported for mixtures of carbon dioxide, water and thermodynamic promoters forming structure II hydrates. Hydrate (H)-aqueous liquid (Lw)-vapour (V) equilibrium pressures for the ternary system composed of water, tetrahydrofuran (THF), and carbon dioxide (CO2), with 5.0 mole percent THF in the initial aqueous phase, are presented in the temperature range from 283.3K to 285.2K. At 283.3K, the three-phase equilibrium pressure is determined to be 0.61MPa (absolute pressure). Four-phase hydrate (H)-aqueous liquid (Lw)-organic liquid (La)-vapour (V) equilibrium data are presented for the ternary system of water-cyclopentane-carbon dioxide at temperatures ranging from 285.2K down to 275.5K. New four-phase H-Lw-La-V equilibrium data for the quaternary system water-THF-cyclopentane-carbon dioxide are presented in the temperature range from 275.1K to 286.6K. It is shown that upon adding THF to the pure aqueous phase to form a 4 mass percent solution, the equilibrium pressure of the formed hydrates may be lowered compared to the ternary system of water, cyclopentane and carbon dioxide. © 2013 Elsevier Ltd.
Thermodynamics of Phase Change Solvents
Use of Water-Oil-Surfactant System Phase Behavior Data/Model for Emulsion-based Chemical Product Design

General information
State: Published
Organisations: Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering, Norwegian University of Science and Technology
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Vapor-Liquid Equilibrium of CO2 with Aqueous Solutions of DEEA, MAPA and their Mixture

General information
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Organisations: Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, CERE – Center for Energy Resources Engineering
Authors: Mattei, M. (Intern), Kontogeorgis, G. (Intern), Gani, R. (Intern)
Number of pages: 2
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Vapor–Liquid-Liquid Equilibrium Measurements and Modeling of Ethanethiol + Methane + Water, 1-Propanethiol + Methane + Water and 1-Butanethiol + Methane + Water Ternary Systems at 303, 335, and 365 K and Pressure Up to 9 MPa

New vapor–liquid–liquid equilibrium (VLLE) data for ethanethiol + methane + water, 1-propanethiol + methane + water, and 1-butanethiol + methane + water ternary systems have been measured at three temperatures (303, 335, and 365 K)
and pressures up to 9 MPa. A “static-analytic” method was used for performing the measurements; the total system pressure was maintained by CH4. The objective of this work is to provide experimental VLLE data for mixtures of mercaptans (thiols) with other natural gas contents at its crude form, for which no data are available in the open literature. Such data will help the industrial modeling of processes relevant to reduction of sulfur emissions. The Cubic-Plus-Association (CPA) equation of state was applied to describe the phase behavior of the investigated systems. It is shown that the CPA EoS satisfactorily describes the solubilities of mercaptans (thiols) in all phases. However, the model underestimates the water content of the vapor phase, especially at low pressures and at the highest investigated temperature, i.e., at 365 K. Only the ethanethiol + methane + water system showed significant cross-association effects.
Waterflooding optimization in uncertain geological scenarios

In conventional waterflooding of an oil field, feedback based optimal control technologies may enable higher oil recovery than with a conventional reactive strategy in which producers are closed based on water breakthrough. To compensate for the inherent geological uncertainties in an oil field, robust optimization has been suggested to improve and robustify optimal control strategies. In robust optimization of an oil reservoir, the water injection and production borehole pressures (bhp) are computed such that the predicted net present value (NPV) of an ensemble of permeability field realizations is maximized. In this paper, we both consider an open-loop optimization scenario, with no feedback, and a closed-loop optimization scenario. The closed-loop scenario is implemented in a moving horizon manner and feedback is obtained using an ensemble Kalman filter for estimation of the permeability field from the production data. For open-loop implementations, previous test case studies presented in the literature, show that a traditional robust optimization strategy (RO) gives a higher expected NPV with lower NPV standard deviation than a conventional reactive strategy. We present and study a test case where the opposite happen: The reactive strategy gives a higher expected NPV with a lower NPV standard deviation than the RO strategy. To improve the RO strategy, we propose a modified robust optimization strategy (modified RO) that can shut in uneconomical producer wells. This strategy inherits the features of both the reactive and the RO strategy. Simulations reveal that the modified RO strategy results in operations with larger returns and less risk than the reactive strategy, the RO strategy, and the certainty equivalent strategy. The returns are measured by the expected NPV and the risk is measured by the standard deviation of the NPV. In closed-loop optimization, we investigate and compare the performance of the RO strategy, the reactive strategy, and the certainty equivalent strategy. The certainty equivalent strategy is based on a single realization of the permeability field. It uses the mean of the ensemble as its permeability field. Simulations reveal that the RO strategy and the certainty equivalent strategy give a higher NPV compared to the reactive strategy. Surprisingly, the RO strategy and the certainty equivalent strategy give similar NPVs. Consequently, the certainty equivalent strategy is preferable in the closed-loop situation as it requires significantly less computational resources than the robust optimization strategy. The similarity of the certainty equivalent and the robust optimization based strategies for the closed-loop situation challenges the intuition of most reservoir engineers. Feedback reduces the uncertainty and this is the reason for the similar performance of the two strategies.

General information
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Pages: 991-1013
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Journal: Computational Geosciences
Wettability of quartz surface as observed by NMR transverse relaxation time ($T_2$)

Injection of optimized water composition (smart water) is an advanced water flooding method for Enhanced Oil Recovery (EOR). Low saline waterflooding has been proved successful in sandstone reservoir. However, there is still controversy on the mechanism of smart water flooding. We studied the wettability property of quartz surface by using Nuclear Magnetic Resonance (NMR) method. The principle of this method is that protons in water relax faster when it comes close to solid surface. We observed that quart is highly water wet. A layer of water (bound water) forms on the quartz surface when they
are mixed. The amount of bound water increases polynomially with increased surface area. Addition of some ions in water based solutions increases the amount of bound water for same amount of surface area. We studied the affect of Ca2+, Mg2+ and Na+ ions and observed that Mg2+ ion produces the maximum amount of bound water while Ca2+ ion produces the least. The result obtained from this study could be used to decide optimized water composition for waterflooding in sandstone reservoirs.

General information
State: Published
Organisations: Department of Civil Engineering, Section for Geotechnics and Geology, Center for Energy Resources Engineering, Section for Structural Engineering
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Workshop on industrial use of molecular thermodynamics

General information
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Organisations: Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering, University of Lorraine, IFP Energies nouvelles
Authors: Kontogeorgis, G. (Intern), Jaubert, J. (Ekstern), de Hemptinne, J. (Ekstern)
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**General information**

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Organisations: Department of Applied Chemistry, Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering, Universite de Lorraine, IFP Energies nouvelles  
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Web of Science (2016): Indexed yes  
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Scopus rating (2014): SJR 0.387 SNIP 0.662 CiteScore 1.27  
BFI (2013): BFI-level 1  
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ISI indexed (2013): ISI indexed yes  
Web of Science (2013): Indexed yes  
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Scopus rating (2012): SJR 0.612 SNIP 1.108 CiteScore 1.56  
ISI indexed (2012): ISI indexed yes  
BFI (2011): BFI-level 1
A Comparative Study of Reduced Variables Based Flash and Conventional Flash

Speeding up flash calculation is a central issue in compositional reservoir simulations since phase equilibrium calculation is the most time-consuming part in those simulations. The reduced variables methods, or the reduction methods, reformulate the original phase equilibrium problem with a smaller set of independent variables. Various versions of the reduced variables methods have been proposed since the mid 80’s. The methods were first proposed for cubic equations of state (EoS) with zero binary interaction parameters (BIPs) and later generalized to situations with non-zero BIP matrices. Most of the studies in the last decade suggest that the reduced variables methods are much more efficient than the conventional flash method. However, Haugen and Beckner questioned the advantages of the reduced variables methods in their recent paper (SPE 141399). A fair comparison between the reduced variables based flash and the conventional flash is not straightforward since the former is difficult to be formulated as unconstrained minimization and involves more complicated composition derivatives. With the recent formulations by Nichita and Graciaa (2010), it is possible to code the reduced variables methods without extensive modifications of Michelsen’s conventional flash algorithm. A minimization based reduced variables algorithm was coded and compared with the conventional minimization based flash. A test using the SPE 3 example showed that the best reduction in time was less than 20% for the extreme situation of 25 components and just one row/column with non-zero BIPs. A better performance can actually be achieved by a simpler implementation directly using the sparsity of the BIP matrix.
A Dantzig-Wolfe Decomposition Algorithm for Linear Economic MPC of a Power Plant Portfolio

Recently, the interest in renewable energy sources is increasing. In the short future, their penetration in the power systems will be significantly higher than today. Denmark is working on achieving its goal by 2020 of having 30% of the energy production provided by renewable sources. 50% of the total power consumption is expected to stem from wind turbines. Due to the inherent stochasticity in renewable energy systems (RES), their energy production is usually complicated to forecast and control. The aim of the smart grid in which consumers as well as producers are controlled is to allow for larger variation in the power production due to the significant amount of renewable energy. The multiple power generators and consumers must be coordinated to balance the supply and demand for power at all times. The aim of this study is to examine a control technique for large scale distributed energy systems (DES), where a significant amount of renewable energy sources are present. Economic Model Predictive Control (MPC) is applied to control the power generators, minimizing the cost and producing the amount of energy required. We examine the large scale scenario, where multiple power generators and consumers such as e.g. electrical vehicles, heat pumps for domestic heating, and refrigeration and cooling systems must be controlled to balance the supply and demand for power. The system is very large scale. To address the large scale of the system and be able to compute the control decisions within a sample period, Dantzig-Wolfe decomposition is used for solution of the resulting linear program describing the Economic MPC of such systems. The controller obtained has been tested by simulations of a power portfolio system.

General information

State: Published
Authors: Standardi, L. (Intern), Edlund, K. (Ekstern), Poulsen, N. K. (Intern), Jørgensen, J. B. (Intern)
Pages: 141
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Publisher: Technical University of Denmark (DTU)
Editors: Jørgensen, J. B., Huusom, J. K., Sin, G.
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A Dantzig-Wolfe Decomposition Algorithm for Linear Economic MPC of a Power Plant Portfolio

Future power systems will consist of a large number of decentralized power producers and a large number of controllable power consumers in addition to stochastic power producers such as wind turbines and solar power plants. Control of such large scale systems requires new control algorithms. In this paper, we formulate the control of such a system as an Economic Model Predictive Control (MPC) problem. When the power producers and controllable power consumers have linear dynamics, the Economic MPC may be expressed as a linear program and we apply Dantzig-Wolfe decomposition for solution of this linear program. The Dantzig-Wolfe decomposition algorithm for Economic MPC is tested on a simulated case study with a large number of power producers. The Dantzig-Wolfe algorithm is compared to a standard linear programming (LP) solver for the Economic MPC. Simulation results reveal that the Dantzig-Wolfe algorithm is faster than the standard LP solver and enables solution of larger problems.

General information

State: Published
Organisations: Center for Energy Resources Engineering, Department of Informatics and Mathematical Modeling, Scientific Computing, Mathematical Statistics
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Number of pages: 8
Publication date: 2012

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Title of host publication: The 10th European Workshop on Advanced Control and Diagnosis (ACD 2012)
A Frequency Matching Method: Solving Inverse Problems by Use of Geologically Realistic Prior Information

The frequency matching method defines a closed form expression for a complex prior that quantifies the higher order statistics of a proposed solution model to an inverse problem. While existing solution methods to inverse problems are capable of sampling the solution space while taking into account arbitrarily complex a priori information defined by sample algorithms, it is not possible to directly compute the maximum a posteriori model, as the prior probability of a solution model cannot be expressed. We demonstrate how the frequency matching method enables us to compute the maximum a posteriori solution model to an inverse problem by using a priori information based on multiple point statistics learned from training images. We demonstrate the applicability of the suggested method on a synthetic tomographic crosshole inverse problem.

General information
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Organisations: Center for Energy Resources Engineering, Department of Informatics and Mathematical Modeling, Scientific Computing, CERE – Center for Energy Resources Engineering
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Pages: 783-803
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Main Research Area: Technical/natural sciences

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Scopus rating (2011): SJR 0.801 SNIP 1.452 CiteScore 1.84
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Scopus rating (2010): SJR 0.822 SNIP 1.273
BFI (2009): BFI-level 1
Analyzing Control Challenges for Thermal Energy Storage in Foodstuffs

We consider two important challenges that arise when thermal energy is to be stored in foodstuffs. We have previously introduced economic optimizing MPC schemes that both reduce operating costs and offer flexible power consumption in a future Smart Grid. The goal is to utilize the thermal capacity of refrigerated goods in a supermarket to shift the load of the system in time without deteriorating the quality of the foodstuffs. The analyses in this paper go before closing any control loops. In the first part, we introduce and validate a new model with which we can estimate the actual temperatures of refrigerated goods from available air temperature measurements. This is based on data obtained from a dedicated experiment. Since limits are specified for food temperatures, the estimate is essential for full exploitation of the thermal potential. Secondly, the thermal properties, shapes and sizes of different foodstuffs make them behave differently when exposed to changes in air temperature. We present a novel analysis based on Biot and Fourier numbers for the different foodstuffs. This provides a valuable tool for determining how different items can be utilized in load-shifting schemes on different timescales and for estimating maximum energy storage time. The results are shown for a large range of parameters, and with specific calculations for selected foodstuff items.

General information
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Organisations: Department of Informatics and Mathematical Modeling, Scientific Computing, Department of Electrical Engineering, Automation and Control, Institute for Product Development, Center for Energy Resources Engineering, Vestas Technology R&D
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Publication: Research - peer-review › Article in proceedings – Annual report year: 2012
A New Comprehensive Approach for Predicting Injectivity Decline during Waterflooding

Injectivity decline during sea waterflooding or produced water re-injection is widely observed in North Sea, Gulf of Mexico and Campos Basin fields. The formation damage occurs mainly due to the deposition of suspended solids around injectors and the build-up the external filter cakes in the well bores. The ability to predict injectivity decline accurately is of great importance for project designs and water management. A comprehensive model that incorporates a variety of factors influencing the process is desirable for the prediction. In this paper, a new comprehensive approach for predicting injectivity decline during water flooding is proposed. The deep bed filtration is described by novel stochastic random walk equations. The injectivity decline model takes into account the reservoir heterogeneity and the distribution of solid particles by sizes. It also accounts for the later formation of the external filter cake and its erosion. A piece of software SNY is developed with the proposed model. The model is able to capture the behaviors of the injectors in the field: the initial slow injectivity decline due to the deep bed filtration of suspended particles, the later faster decline due to the build-up of the external cake, and the temporary steady state due to the cake erosion. Stronger normal dispersion or median heterogeneity close to the injector leads to farther penetration of the particles and slower impedance increase. Neglecting the particle population heterogeneity may lead to the underestimation of formation damage and predicts late transition to external cake formation. The impedance at the steady state and the starting time are highly influenced by the cake properties. The impedance and the external cake thickness at the steady state are likely to be higher in horizontal wells than those in vertical wells.

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Organisations: Center for Energy Resources Engineering, CERE – Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, University of Adelaide
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Application of simplified PC-SAFT to glycol ethers
The simplified PC-SAFT (sPC-SAFT) equation of state is applied for binary glycol ether-containing mixtures, and it is investigated how the results are influenced by inclusion of intramolecular association in the association theory. Three different glycol ethers are examined: 2-methoxyethanol, 2-ethoxyethanol, and 2-butoxyethanol. Vapor-liquid and liquid-liquid equilibria of miscible and immiscible, self- and cross-associating mixtures are considered, including the closed-loop liquid-liquid equilibrium of 2-butoxyethanol-water. The results are finally compared to other association models. © 2011 American Chemical Society.

General information
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Organisations: Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering, CERE – Center for Energy Resources Engineering
Authors: Avlund, A. S. (Intern), Kontogeorgis, G. (Intern), Michelsen, M. L. (Intern)
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Application of Stochastic Approaches to Modelling Suspension Flow in Porous Media

The goal of this chapter is to overview several stochastic approaches to modelling suspension flows in porous media, including the population balance approach, the continuous time random walk (CTRW) approach, and its reduction to the elliptic equation approach. Most of these approaches emerged recently, although their mathematical background is relatively well known. Some problems (like upscaling) require the development of new methods. The connections between the formalisms, the discrepancies between them and their capabilities are analysed and compared. Comparison to experimental data is also briefly discussed. The population balance models growing out of the Boltzmann-Smolukhowski formalism take into account the particle and the pore size distributions. A system of integral-differential kinetic equations for the particle transport is derived and averaged. The continuous-time random walk theory considers the distribution of the residence times of particles in pores. The transport equation derived in the framework of CTRW contains a convolution integral with a memory kernel accounting for the particle flight distribution. An important simplification of the CTRW formalism, its reduction to an elliptic transport equation, is also discussed. The CTRW approach and the elliptic equation are both able to catch abnormal behaviour of suspended particles, such as the algebraic decaying tail in the breakthrough curve or asymmetric particle distribution from a pulse injection. The elliptic equation approach can be generalized onto polydisperse particle and pore systems, just incorporating the characteristic features and advantages of both CTRW and population balance approaches.

General information

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Authors: Shapiro, A. (Intern), Yuan, H. (Intern)
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Application of the UNIFAC-CI Model for Phase Equilibria Predictions of Organic Chemical System

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Authors: Mustaffa, A. A. (Intern), Kontogeorgis, G. (Intern), Gani, R. (Intern)
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Approach to Improve Speed of Sound Calculation within PC-SAFT Framework

An extensive comparison of SRK, CPA and PC-SAFT for speed of sound in normal alkanes has been performed. The results reveal that PC-SAFT captures the curvature of speed of sound better than cubic EoS but the accuracy is not
satisfactory. Two approaches have been proposed to improve PC-SAFT’s accuracy for speed of sound: (i) putting speed of sound data into parameter estimation; (ii) putting speed of sound data into both universal constants regression and parameter estimation. The results have shown that the second approach can significantly improve the speed of sound (3.2%) prediction while keeping acceptable accuracy for the primary properties, i.e. vapor pressure (2.1%) and liquid density (1.5%). The two approaches have also been applied to methanol, and both give very good results.

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Authors: Liang, X. (Intern), Maribo-Mogensen, B. (Intern), Thomsen, K. (Intern), Yan, W. (Intern), Kontogeorgis, G. (Intern)
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BFI (2008): BFI-level 2
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Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.105 SNIP 1.239
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We, herein, present a statistical method for diagnostics of the outliers in phase equilibrium data (dissociation data) of simple clathrate hydrates. The applied algorithm is performed on the basis of the Leverage mathematical approach, in which the statistical Hat matrix, Williams Plot, and the residuals of a selected correlation results lead to define the probable outliers. This method not only contributes to outliers diagnostics but also identifies the range of applicability of the applied model and quality of the existing experimental data. The available correlation in the literature in exponential form is used to represent/predict the hydrate dissociation pressures for three-phase equilibrium conditions (liquid water/ice–vapor–hydrate). The investigated hydrate formers are methane, ethane, propane, carbon dioxide, nitrogen, and hydrogen sulfide. It is interpreted from the obtained results that the applied correlation for calculation/estimation of the phase behavior of simple clathrate hydrate systems is statistically valid and correct, 5 hydrate dissociation data are found to be probable doubtful ones and 10 data points are out of applicability domain of the applied correlation.
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Web of Science (2004): Indexed yes
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Web of Science (2003): Indexed yes
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Highlights:
- Leverage method is applied for evaluation of experimental phase equilibrium data.
- Experimental phase equilibrium data of various simple clathrate hydrates are studied.
- 5 hydrate dissociation data are found to be probable doubtful ones.
A Systematic Methodology for Design of Emulsion Based Chemical Products

A systematic methodology for emulsion based chemical product design is presented. The methodology employs a model-based product synthesis/design stage and a model-experiment based further refinement and/or validation stage. In this paper only the first stage is presented. The methodology employs a hierarchical approach starting with the identification of the needs to be satisfied by the emulsified product and then building up the formulation by adding one-by-one the different classes of chemicals. A structured database together with dedicated property prediction models and evaluation criteria are employed to obtain a list of formulations that satisfy constraints representing the desired needs (target properties). Through a conceptual case study dealing with the design of a sunscreen lotion, the application of this new methodology is illustrated.

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A Systematic Methodology for Design of Emulsion Based Chemical Products

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Calculation of minimum miscibility pressure using fast slimtube simulation
Minimum miscibility pressure (MMP) is a critical parameter in designing a miscible gas injection process. It is expected that 100% displacement efficiency on the microscopic scale can be achieved provided the injection pressure is above MMP. Two approaches are usually employed for equation of state (EoS) based MMP calculation. The slimtube simulation approach is a numerical simulation of the physical slimtube experiment, which is commonly accepted as the most reliable experimental method for MMP determination. This approach carries out slimtube simulation runs at a series of pressures and determines the MMP from the recovery-pressure curve, just as in the experiment. The global approach, which is based on the method of characteristics analysis of 1D gas injection, finds the MMP by locating the pressure where a key tie-line becomes critical. Although the global approach is faster, the slimtube approach is still a necessary complementary method especially when the injection process involves complex phase behavior caused by CO2 or heavy oils. This study addresses how to improve the computational efficiency of slimtube simulation for MMP calculation. Firstly, a robust and
efficient algorithm for rigorous flash forms the basis of the whole strategy. Secondly, a tie-line distance based approximation (TDBA) method has been introduced on top of the rigorous algorithm. In the TDBA method, if a new feed composition in a grid block is close enough to a tie-line previously calculated in the same block, the previous tie-line results can be used with slight adjustment. The approximation affects the final recovery very little but greatly increases the speed. Thirdly, a higher order method can be employed to use a fewer number of grid blocks to get the same accuracy in recovery. Finally, a MMP search strategy is proposed to reduce the number of slimtube simulations needed. In addition, it is also discussed how to parallelize slimtube simulations for modern computers with multiple CPU cores to further chop the computation time. Copyright 2012, Society of Petroleum Engineers.

General information
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Capabilities and Limitations of an Association Theory for Chemicals in Liquid or Supercritical Solvents
The cubic-plus-association (CPA) model is an equation of state (EoS) that combines the Soave–Redlich–Kwong (SRK) equation with the association term from Wertheim’s theory as used in statistical associating fluid theory (SAFT). In the form used here, the CPA EoS does not include separate terms for the polar and quadrupolar contributions. The capabilities and limitations of the CPA model when it is applied to mixtures with nonpolar and polar chemicals, as well as associating (hydrogen-bonding) compounds are illustrated. Three case studies are considered, all of which are of industrial relevance. The capabilities of the model are illustrated in the first two case studies: the phase behavior of mixtures used in the oxidation of 2-octanol in supercritical CO2 and the investigation of systems containing acetone, methanol, water, chloroform, and methyl acetate. In each case, both correlations of vapor–liquid and liquid–liquid equilibria for binary systems and predictions for multicomponent mixtures are presented. Finally, the limitations of the CPA model are illustrated in the last case study, which focuses on the modeling of mixtures containing aromatic acids, such as benzoic and terephthalic acid. We also include a detailed discussion of the capabilities and limitations of the model in context and related to previous investigations. Finally, results are compared to observations from studies with other association models.

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Chalk as a reservoir

Reservoir properties of chalk depend on the primary sediment composition as well as on subsequent diagenesis and tectonic events. Chalks of the North Sea almost exclusively have mudstone or wackestone texture. Microfossils may have retained their porosity where degree of diagenesis is low, or be partly or fully cemented where diagenesis is more pronounced. It is a chalk characteristic that permeability is controlled by the porosity and internal surface of the mud matrix, whereas the larger pores play an insignificant role. Cemented microfossils may take up a significant volume in a wackestone, and the best reservoir properties are typically found in mudstone intervals.

Chalk mudstones vary a lot though. The best mudstones are purely calcitic, well sorted and may have been redeposited by traction currents. Other mudstones are rich in very fine grained silica, which takes up pore space and thus reduces porosity at the same time as it increases specific surface and thus cause permeability to be low. In the Central North Sea the silica is quartzitic. Silica rich chalk intervals are typically found in the Ekofisk and Hod formations. In addition to silica, Upper Cretaceous and Palaeogene chalks typically contain small amounts of clay minerals. Chalk of the Lower Cretaceous Tuxen Formation can contain so much clay that it has a negative effect on the reservoir properties.

With respect to solid volume a chalk may contain more than 95% calcite, but the internal surface of the same chalk may be only 50% calcite, leaving the remaining internal surface to the fine grained silica and clay. The high specific surface of these components causes clay- and silica rich intervals to have high irreducible water saturation. Although chalks typically are found to be water wet, chalk with mixed wettability is reported, possibly as a reflection of the mixed mineralogy of the internal surface. Internal surface thus varies stratigraphically, but it also varies among hydrocarbon reservoirs, possibly reflecting a varying temperature. This is because the biogenic calcite making up the chalk, subsequent to deposition stabilizes chemically by recrystallization. This process requires energy and is promoted by temperature. This recrystallization in principle does not influence porosity, but only specific surface, which decreases during recrystallization, causing permeability to increase. The central North Sea is a warm basin, so stylolite formation in the chalk is controlled by effective burial stress. The stylolites are zones of calcite dissolution and probably are the source of calcite for porefilling cementation which is typical in water zone chalk and also affect the reservoirs to different extent. The relatively high porosity in hydrocarbon reservoirs can be a result of hydrocarbon emplacement quenching stylolites and stopping or retarding pressure dissolution.

In some chalk reservoir intervals, hydrocarbon emplacement has been so early that the reservoirs are practically uncemented. These reservoir intervals have hardly any stylolites and can have porosity above 40% or even 50% and thus also have relatively high permeability. Such intervals have the problem though, that increasing effective stress caused by hydrocarbon production results in mechanical compaction and overall subsidence. Most other chalk intervals are to some extent cemented and cannot compact mechanically at realistic effective stresses and only deform elastically. All chalk intervals though, may react by fracturing to changes in shear stress. So where natural fractures are not prevalent, fractures may be generated hydraulically. Fractures play a significant role in the production of hydrocarbons from chalk reservoirs.

Change of Static and Dynamic Elastic Properties due to CO² Injection in North Sea Chalk

Reservoir modeling and monitoring uses dynamic data for predicting and determining static changes. Dynamic data are achieved from the propagation velocity of elastic waves in rock while static data are obtained from the mechanical deformation. Reservoir simulation and monitoring are particularly important in enhanced oil recovery by CO₂ injection (CO₂-EOR) in chalk as, chalk reservoirs are vulnerable to compaction under changed stress and pore fluid. From South Arne field, North Sea, we used Ekofisk Formation chalk having approximately 20% non-carbonate and Tor Formation chalk having less than 5% non-carbonate. We studied difference in static and dynamic behavior. Furthermore, brine saturated data were compared with CO₂ injected data to reveal the effect of supercritical CO₂ injection in both static and dynamic elastic properties. We used strain gauges and LVDTs to measure static deformation. We observed lower dynamic elastic modulus for chalk with higher non-carbonate content at porosities lower than 30%. In 30% porosity chalk, dynamic compressional and bulk modulus were found significantly higher than the static modulus. Static measurements with LVDT were found lowest. The effect of CO₂ injection was notable in dynamic elastic properties, while a possible change in static elastic properties was below detection limit.
Comparing ignitability for in situ burning of oil spills for an asphaltenic, a waxy and a light crude oil as a function of weathering conditions under arctic conditions

In situ burning of oil spills in the Arctic is a promising countermeasure. In spite of the research already conducted more knowledge is needed especially regarding burning of weathered oils. This paper uses a new laboratory burning cell (100 mL sample) to test three Norwegian crude oils, Grane (asphaltenic), Kobbe (light oil) and Norne (waxy), for ignitability as a function of ice conditions and weathering degree. The crude oils (9 L) were weathered in a laboratory basin (4.8 m3) under simulated arctic conditions (0, 50 and 90% ice cover). The laboratory burning tests show that the ignitability is dependent on oil composition, ice conditions and weathering degree. In open water, oil spills rapidly become "not ignitable" due to the weathering e.g. high water content and low content of residual volatile components. The slower weathering of oil spills in ice (50 and 90% ice cover) results in longer time-windows for the oil to be ignitable. The composition of the oils is important for the window of opportunity. The asphaltenic Grane crude oil had a limited time-window for in situ burning (9 h or less), while the light Kobbe crude oil and the waxy Norne crude oil had the longest time-windows for in situ burning (from 18 h to more than 72 h). Such information regarding time windows for using in situ burning is very important for both contingency planning and operational use of in situ burning.
Comparison of the Debye–Hückel and the Mean Spherical Approximation Theories for Electrolyte Solutions

The thermodynamics of electrolyte solutions has been investigated by many scientists throughout the last century. While several theories have been presented, the most popular models for the electrostatic interactions are based on the Debye–Hückel and mean spherical approximation (MSA) theories. In this paper we investigate the differences between the Debye–Hückel and the MSA theories, and comparisons of the numerical results for the Helmholtz energy and its derivatives with respect to temperature, volume and composition are presented. The investigation shows that the nonrestricted primitive MSA theory performs similarly to Debye–Hückel, despite the differences in the derivation. We furthermore show that the static permittivity is a key parameter for both models and that in many cases it completely dominates the results obtained from the two models. Consequently, we conclude that the simpler Debye–Hückel theory may be used in connection with electrolyte equations of state without loss of accuracy.

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Comparison of two electrolyte models for the carbon capture with aqueous ammonia

Post-combustion carbon capture is attracting much attention due to the fact that it can be retrofitted on existing coal power plants. Among the most interesting technologies is the one that employs aqueous ammonia solutions to absorb the generated carbon dioxide. The evaluation of such process requires the modeling of electrolyte solutions. In this work two thermodynamic models for electrolyte solutions are compared against each other with respect to experimental data. They are the e-NRTL model and the Extended UNIQUAC model, both implemented in the commercial software Aspen Plus®1 (version 7.2). Subsequently, a simple absorption/regeneration layout is simulated employing both models and the process performances are compared. In general, the Extended UNIQUAC appears to describe the experimental data for larger ranges of temperature, pressure and concentration of ammonia more satisfactorily. The energy performances computed with the Extended UNIQUAC models are less promising than with the e-NRTL model.
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Control of Blood Glucose for People with Type 1 Diabetes: an In Vivo Study
Since continuous glucose monitoring (CGM) technology and insulin pumps have improved recent years, a strong interest in a closed-loop artificial pancreas for people with type 1 diabetes has arisen. Presently, a fully automated controller of blood glucose must face many challenges, such as daily variations of patient's physiology and lack of accuracy of glucose sensors. In this paper we design and discuss an algorithm for overnight closed-loop control of blood glucose in people with type 1 diabetes. The algorithm is based on Model Predictive Control (MPC). We use an offset-free autoregressive model with exogenous input and moving average (ARMAX) to model the patient. Observer design and a time-varying glucose reference signal improve robustness of the algorithm. We test the algorithm in two clinical studies conducted at Hvidovre Hospital. The first study took place overnight, and the second one took place during daytime. These trials demonstrate the importance of observer design in ARMAX models and show the possibility of stabilizing blood glucose during the night.

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Control of Blood Glucose for People with Type 1 Diabetes: an In Vivo Study

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CO₂ Capture from Flue gas using Amino acid salt solutions

By implementing carbon dioxide (CO₂) capture, it is possible to clean the flue gas from coal-fired power plants, so that it is almost completely free of this greenhouse gas. The most advanced techniques towards practical application are based on chemical absorption, where CO₂ in the flue gas is chemically bond by a solvent, usually an aqueous solution of amines, resulting in a cleaned gas being released to the atmosphere. Heating of the solution, desorbs the CO₂ and regenerates the solvent, which is then ready for a new round of absorption. The captured CO₂ can then be compressed and sent to storage.

Typical solvents for the process are based on aqueous solutions of alkanolamines, such as mono-ethanolamine (MEA), but their use implies economic disadvantages and environmental complications. Amino acid salt solutions have emerged as an alternative to the alkanolamines, partly because they are naturally occurring substances, and partly because they have desirable properties, such as lower vapor pressures and higher stability against oxidative degradation. One important feature of these new solvents is the formation of solids upon CO₂ absorption, which happens especially at higher CO₂ loadings and/or amino acid salt concentrations. The formation of solids poses challenges, but it also holds the promise for improving the efficiency of the capture process.

This project focuses on phase equilibrium experiments of five systems CO₂ + amino acid salt + H₂O, at conditions relevant for the CO₂ capture process. Also, attention is given to the chemical compositions of the precipitations, which forms as a result of CO₂ absorption into the five amino acid salt solutions.

Phase equilibrium data are needed to develop safe and economically viable capture processes. Two different experimental apparatuses were used. One was developed specifically for this project and is based on an analytical semi-flow method. The other has recently been developed in another project, and is based on a synthetic method. The semi-flow method was used for measurements at 10 kPa CO₂ partial pressure, total pressure equal to the atmospheric pressure and temperatures of 298 K, 313 K and 323 K; these conditions cover the absorber part of the capture process. The apparatus based on the synthetic method was used to obtain data at different pressures and temperatures up to 353 K (80 ºC), which is the maximum operation temperature of some of the components in the apparatus. Ideally, measurements in the full temperature range for desorption, which usually needs approximately 393 K (120 ºC), would be desirable.

Using the 2 apparatuses, CO₂ solubility in aqueous solutions of MEA and the potassium salts of taurine, glycine, L-alanine, L-proline and L-lysine were examined. It was found that all of the tested amino acid salt solutions have the potential to replace MEA. Nevertheless, solutions of the potassium salt of L-lysine showed the best properties.

The chapters of this thesis are organized as follows:

Chapter 1 is a brief introduction to the central issues of this work, setting the subject of the project in perspective to the issues of global warming and CO₂ capture and storage (CCS).

Chapter 2 explains the principle behind the chemical absorption of CO₂ from flue gas, emphasizing on the issues involving the solvent.

Chapter 3 is dedicated to the concept of using amino acids salt solutions as solvents in CO₂ capture, it includes a description of general amino acids chemistry and an outline of the chemical reactions involved in CO₂ absorption into amino acids salt solutions.

Chapter 4 deals with the description and validation of the new apparatus for measuring of CO₂ solubility based on the semi-flow method. A validation study of CO₂ solubility in aqueous solutions of MEA is presented.

Chapter 5 focuses on the determination of the chemical compositions of the precipitations, which arise in the five amino acid salt solutions upon CO₂ absorption. The solutions were saturated with CO₂ at 298 K, using the apparatus based on the semi-flow method. The precipitates were isolated and analyzed with XRD.

Chapter 6 concerns a CO₂ solubility study using the apparatus based on the semi-flow method; CO₂ solubility were examined in aqueous solutions of MEA and the five amino acid salts, with concentrations between 2 and 8 molal and...
temperatures around 298 K, 333 K and 323 K. Chapter 7 describes a CO$_2$ solubility study using the apparatus based on the synthetic method; CO$_2$ solubility in aqueous solutions of the potassium salts of Lysine and L-proline, with concentrations of 3.5 molal and 7 molal respectively, were studied at CO$_2$ partial pressures up to about 760 kPa, and temperatures around 313 K, 333 K and 353 K. Similar data were obtained with solutions of 7 molal MEA, at the same temperatures and at CO$_2$ partial pressures up to around 2.3 MPa.

Chapter 8 concludes on the accomplishments of the project, and finally addresses considerations concerning future work.
Determining Upper Bounds for the Clay-squirt Effect in Clay Bearing Sandstone

Sonic measurements of saturated bulk moduli of clay bearing sandstones show larger values than expected by Gassmann modelling from dry rock properties. This causes difficulties in extrapolation of laboratory data to different saturants or frequencies. Squirt flow from the clay phase of the rock have been proposed as the mechanism behind this stiffening. Low fluid mobility and low bulk modulus of the clay phase cause excess pore-pressures to be induced and retained in the phase leading to stiffening. A quantitative bound is formulated for this effect through the determination of the Hashin-Shtrikman bounds for the case of a drained clay phase and an undrained clay phase. The bound is achieved by analyzing the influence of the relevant parameters with subsequent grouping using reasonable correlations. Through this approach only the saturated bulk modulus of the quartz phase and the clay fraction remain as free parameters. The bound is calculated for all possible values of these parameters. Experimentally observed values for non-Gassmann bulk modulus stiffening are found to fall below the bound for all values within the Hashin-Shtrikman bounds. Hereby this study shows that the clay-squirt effect may be the cause of observed stiffening.

Development and Analysis of Original UNIFAC-CI and Modified UNIFAC-CI Models for Prediction of VLE and SLE Systems

Prediction of properties is important in chemical process-product design. Group-contribution (GC) methods provide useful tool but there is a need to validate and improve their accuracy when complex chemicals are present in the mixtures. In accordance with that, a combined GC and atom connectivity approach that is able to extend the application range of property models has been developed for mixture properties. This so-called GCPlus approach is a hybrid model which combines GC and valence connectivity indices (CI). The main idea is the use of CI to describe the molecular fragmentation that relates properties, the molecular interactions with the molecular structures. One established GC method is the UNIFAC model to predict liquid phase activity coefficients. The needed values of the group interaction parameters (GIPs) are obtained by fitting phase equilibrium data. There are many gaps in the UNIFAC parameter table due to lack of data. Alternative to performing measurements, values of the missing GIPs, can be predicted through the GCPlus approach. The predicted values for the GIPs are then used in the UNIFAC model to calculate activity coefficients. In this work, the model parameters for the GCPlus approach to the original UNIFAC and Modified (Dortmund) UNIFAC have been regressed against vapor-liquid equilibrium (VLE) data and simultaneously against VLE and solid-liquid equilibrium (SLE) data for groups formed by C, H, O, N, Cl and S atoms. Initially the VLE data used to regress these parameters are checked using a quality assessment algorithm which combines four widely used consistency tests (Herington, Van Ness, Point/Differential and Infinite Dilution tests) and also a check on the consistencies of the data with the pure component vapor pressures. The overall quality factors, QVLE obtained for each dataset indicate the quality of each datasets and can then be used as weighting factors, in the objective function for the parameter regression with VLE data (and with SLE data). The performance of the CI-models using parameters regressed against VLE data and simultaneously against VLE and SLE data are compared in terms of the uncertainties of the parameters regressed against the predicted properties and the accuracy of the predictions. In addition, the model performances are compared with their reference UNIFAC models.
Development and testing of a new apparatus for the measurement of high-pressure low-temperature phase equilibria

A new apparatus for the study of high-pressure phase equilibria at low temperatures using an analytical method was designed, assembled and tested. The apparatus was specially developed for the study of multi-phase equilibria in systems containing hydrocarbons, water and hydrate inhibitors, at temperatures ranging from 213K to 353K and pressures up to 40MPa. The core of the apparatus is a variable-volume equilibrium cell, equipped with a 360° sapphire window and connected to an analytical system by three capillary samplers. The quality of the apparatus was confirmed through several tests, including the study of the system methane+water. An equilibrium point for the quaternary system methane+n-hexane+methanol+water is also presented.

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Development of a group contribution method for determination of viscosity of ionic liquids at atmospheric pressure

In this study, a wide literature survey has been carried out to collect an extensive set of liquid viscosity data for ionic liquids (ILs). A data set consisting of 1672 viscosity values and comprising 443 ILs was collated from 204 different literature sources. Using this data set, a reliable group contribution method has been developed. The method employs a total of 46 sub-structures in addition to the temperature to predict the viscosity of ILs. In order to differentiate the effects of the anion and cation on the viscosity of ILs, 24 sub-structures related to the chemical structure of anions, and 22 sub-structures related to the chemical structure of cations were implemented. The proposed model produces a low average relative deviation (AARD) of less than 6.4% taking into consideration all 1672 experimental data values.

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Diagnosis of asphaltene stability in crude oil through "two parameters" SVM model

Asphaltene precipitation/deposition and its imposing difficulties are drastic issues in petroleum industry. Monitoring the asphaltene stability conditions in crude oil systems is still a challenge and has been subject of many studies. In this work, the Refractive Index (RI) of several oil samples is determined using the existing SARA fractions experimental data for this purpose. The powerful Least-Square modification of Support Vector Machine (LSSVM) strategy is applied to develop a computer program, by which the asphaltene stability region can be determined for various crudes. The developed two-parameter model results show 0.6% average absolute relative deviation from the corresponding RI experimental values, measured at 293.15 K and atmospheric pressure, and squared correlation coefficient of 0.722. In the final analysis, a comparison is implemented between the obtained results of the model and previously-presented empirical correlations available in open literature. © 2012 Elsevier Ltd.
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Highlights.
- A new method of monitoring the asphaltene stability in crude oil is developed
- Least-Square Support Vector Machine (LSSVM) is applied for this purpose.
- SARA fraction and Refractive Index data are employed for its development
- Developed two-parameter model results show 0.6% AARD from the RI data.
- A computer program is presented as a predictive tool for detection of the stability.

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Different Methods of Predicting Permeability in Shale
Permeability is often very difficult to measure or predict in shale lithology. In this work we are determining shale permeability from consolidation tests data using Wissa et al., (1971) approach and comparing the results with predicted permeability from Kozeny’s model. Core and cuttings materials were obtained from Fjerritslev shale Formation in Jurassic interval of Stenlille and Vedsted on-shore wells of Danish basin. The calculated permeability from specific surface and porosity vary from 0.09 to 48.53 μD while that calculated from consolidation tests data vary from 1000 μD at a low vertical effective stress to 9 μD at high vertical effective stress of 100 MPa. The indirect permeability calculated from consolidation tests falls in the same magnitude at higher vertical effective stress, above 40 MPa, as that of the Kozeny model for shale samples with high non-clay content ≥ 70% but are higher by two to five orders of magnitudes at lower vertical effective stress below 40 MPa as the content of clay minerals increases causing heterogeneity in shale material. Indirect permeability from consolidation can give maximum and minimum values of shale permeability needed in simulating fluid flow in shale useful in assessing their integrity for CO2 storage, gas shale exploitation and other engineering applications.
Economic Model Predictive Control for Building Climate Control in a Smart Grid

Model Predictive Control (MPC) can be used to control a system of energy producers and consumers in a Smart Grid. In this paper, we use heat pumps for heating residential buildings with a floor heating system. We use the thermal capacity of the building to shift the electricity consumptions to periods with low energy prices. In this way the heating system of the house becomes a flexible power consumer in the Smart Grid. This scenario is relevant for systems with a significant share of stochastic energy producers, e.g. wind turbines, where the ability to shift power consumption according to production is crucial. We present a model for a house with a heat pump used for supplying thermal energy to a floor heating system. The model is a linear state space model and the resulting controller is an Economic MPC formulated as a linear program. The model includes forecasts of both weather and electricity price. Simulation studies demonstrate the capabilities of the proposed model and algorithm. Compared to traditional operation of heat pumps with constant electricity prices, the optimized operating strategy saves 25-33% of the electricity cost.

Effective stress coefficient for uniaxial strain condition

The effective stress coefficient, introduced by Biot, is used for predicting effective stress or pore pressure in the subsurface. It is not a constant value. It is different for different types of sediment and it is stress dependent. We used a model, based on contact between the grains to describe the reason for change in effective stress coefficient under stress. Our model suggests that change in effective stress coefficient will be higher at uniaxial stress condition than at hydrostatic condition. We derived equations from the original definition of Biot to estimate effective stress coefficient from one dimensional rock mechanical deformation. We further investigated the effect of boundary condition on the stress dependency of effective stress coefficient and discussed its application in reservoir study. As stress field in the reservoirs are most unlikely to be hydrostatic, effective stress determined under uniaxial strain condition will be more relevant in reservoir studies.
Effective stress coefficient for uniaxial strain condition

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Effect of Fluid Dynamic Viscosity on the Strength of Chalk

The mechanical strength of high porosity and weakly cemented chalk is affected by the fluid in the pores. In this study, the effect of the dynamic viscosity of non-polar fluids has been measured on outcrop chalk from Sigerslev Quarry, Stevns, Denmark. The outcome is that the measured strength of the chalk decreases with increasing dynamic viscosity. The proposed qualitative explanation is that pressure difference supports and enhances the generation of microscopic shear and tensile failures.
Effect Of Hot Water Injection On Sandstone Permeability: An Analysis Of Experimental Literature

The seasonal imbalance between supply and demand of renewable energy requires temporary storage, which can be achieved by hot water injection in warm aquifers. This requires that the permeability and porosity of the aquifer are not reduced significantly by heating.

We present an overview of published results regarding the effect of temperature on sandstone permeability. These tests are performed with mineral oil, nitrogen gas, distilled water and solutions of NaCl, KCl, CaCl₂ as well as brines that contain a mixture of salts. Thirteen sandstone formations, ranging from quartz arenites to formations with a significant fraction of fine particles including clay minerals are investigated. The porosities range from 0.10 to 0.30 and permeabilities span the range from 1 to 1000 md. To compare different rock types, specific surface is determined from permeability and porosity using Kozeny's equation.

Heating causes thermal expansion, which results in porosity reduction if the sandstone is confined. The maximum effect of porosity reduction as a result of thermal expansion on permeability is modelled and compared the change in specific surface that is computed from the reported data. This does not account for all the permeability reductions observed. Permeability reduction occurs both when distilled water is the saturating fluid as well as in tests with NaCl, KCl or CaCl₂ solutions, however, this is not the case in tests with mineral oil or nitrogen gas. The formation of a filter cake or influx of colloidal particles due to corrosion of the apparatus at elevated temperature causes permeability reduction in a number of investigations. Mobilisation of internal particles, particularly kaolinite particles, is considered a probable mechanism of permeability reduction for the other experiments reviewed here.

The parameters that strongly affect the success of heat storage therefore include the quality of the equipment and particularly the prevention of corrosion, as well as the sandstone lithology and its interaction with the reservoir fluid.

Effects of Everyday Life Events on Glucose, Insulin, and Glucagon Dynamics in Continuous Subcutaneous Insulin Infusion–Treated Type 1 Diabetes: Collection of Clinical Data for Glucose Modeling

Background: In the development of glucose control algorithms, mathematical models of glucose metabolism are useful for conducting simulation studies and making real-time predictions upon which control calculations can be based. To obtain type 1 diabetes (T1D) data for the modeling of glucose metabolism, we designed and conducted a clinical study.

Methods: Patients with insulin pump–treated T1D were recruited to perform everyday life events on two separate days. During the study, patients wore their insulin pumps and, in addition, a continuous glucose monitor and an activity monitor to estimate energy expenditure. The sequence of everyday life events was predetermined and included carbohydrate intake, insulin boluses, and bouts of exercise; the events were introduced, temporally separated, in different orders and in different quantities. Throughout the study day, 10-min plasma glucose measurements were taken, and samples for plasma insulin and glucagon analyses were obtained every 10 min for the first 30 min after an event and subsequently every 30 min.

Results: We included 12 patients with T1D (75% female, 34.3±9.1 years old [mean±SD], hemoglobin A1c 6.7±0.4%). During the 24 study days we collected information-rich, high-quality data during fast and slow changes in plasma glucose following carbohydrate intake, exercise, and insulin boluses. Conclusions: This study has generated T1D data suitable for glucose modeling, which will be used in the development of glucose control strategies. Furthermore, the study has given new physiologic insight into the metabolic effects of carbohydrate intake, insulin boluses, and exercise in continuous subcutaneous insulin infusion–treated patients with T1D.
Electric vehicle charge planning using Economic Model Predictive Control

Economic Model Predictive Control (MPC) is very well suited for controlling smart energy systems since electricity price and demand forecasts are easily integrated in the controller. Electric vehicles (EVs) are expected to play a large role in the future Smart Grid. They are expected to provide grid services, both for peak reduction and for ancillary services, by absorbing short term variations in the electricity production. In this paper the Economic MPC minimizes the cost of electricity consumption for a single EV. Simulations show savings of 50–60% of the electricity costs compared to uncontrolled charging from load shifting based on driving pattern predictions. The future energy system in Denmark will most likely be based on renewable energy sources e.g. wind and solar power. These green energy sources introduce stochastic fluctuations in the electricity production. Therefore, energy should be consumed as soon as it is produced to avoid the need for energy storage as this is expensive, limited and introduces efficiency losses. The Economic MPC for EVs described in this paper may contribute to facilitating transition to a fossil free energy system.

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Equation of state modelling of systems with ionic liquids: Literature review and application with the Cubic Plus Association (CPA) model

For the last decade ionic liquids have been regarded as compounds of interest by the academic and industrial communities. These compounds present several advantages when compared to other typical solvents. However, because of their novelty, a deep understanding of their phase behaviour and their interactions with other components is still needed. In this work, we made a review of literature studies on modelling systems with ionic liquids using equation of state models. Furthermore, we applied the Cubic Plus Association (CPA) equation of state to describe the phase behaviour of two ionic liquids, 1-ethyl-3-methylimidazolium bis(trifluoromethylsulfonylimide ([C2mim][NTf2]) and 1-butyl-3-methylimidazolium bis(trifluoromethylsulfonylimide ([C4mim][NTf2]). The first step was to study an adequate approach for the determination of pure component parameters for the ionic liquids. The parameters were obtained by fitting the predictions of the model to experimental vapour pressure and liquid density data. The parameters provide a good description of both experimental vapour pressures and liquid density, with maximum percentage deviations of respectively 8.9 and 1.3% for [C2mim][NTf2] and 5.7 and 0.5% for [C4mim][NTf2]. Different sets of pure component parameters for each ionic liquid were considered and their suitability to describe the behaviour of ionic liquids was evaluated by modelling the vapour-liquid equilibria (VLE) of mixtures with CO2 and the liquid-liquid equilibria (LLE) with water. The results for VLE proved to be very good in the range of pressures studied when using one temperature-independent binary interaction parameter, with percentage deviations in pressure between 8 and 13% for [C2mim][NTf2] and around 12% for [C4mim][NTf2]. For the LLE of ionic liquids with water a temperature-independent binary interaction parameter was also used, but the results do not describe the experimental data as well as with the VLE, with percentage deviations ranging from 4 to 100%. However, for some of the sets of pure component parameters a good description of the experimental data is obtained and work is in progress for improving the modelling of LLE with the CPA equation of state.

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In this paper, laboratory challenge tests are carried out under unfavorable attachment conditions, so that size exclusion or straining is the only particle capture mechanism. The experimental results show that far above the percolation threshold the filtration coefficients are not proportional to the fractional flow through the pores smaller than the particles, but to the power-law functions of them. The experimental penetration depths of particles can be over thousands of pores even if the particle sizes are comparable to the average pore size. This observation cannot be explained by the traditional size exclusion theory or the model of parallel tubes with mixing chambers, where the filtration coefficients are proportional to the flux through smaller pores, and the predicted penetration depths are much lower. A special capture mechanism is proposed, which makes it possible to explain the experimentally observed power law dependencies of filtration coefficients and large penetration depths of particles. Such a capture mechanism is realized in a 2D pore network model with periodical boundaries with the random walk of particles on the percolation lattice. Geometries of infinite and finite clusters formed by pores of the sizes exceeding the particle size are analyzed with regard to the possibility for particle capture. Two power laws are proposed to describe the filtration coefficients close and far away from the percolation threshold of the lattice. They can be applied to match the filtration coefficients from the network model well while one of them is used to match the experimental results. The application of such a model may lead to more accurate inverse determination of the pore size distributions from the challenge tests.
Evaluating the impact of an ammonia-based post-combustion CO₂ capture process on a steam power plant with different cooling water temperatures

The use of aqueous ammonia is a promising option to capture carbon dioxide from the flue gas of coal-fired power plants. Compared to a capture process using monoethanolamine (MEA), the use of ammonia can reduce the heat requirement of the CO₂ desorption significantly, although an additional effort is necessary to provide the cooling of the process. To allow for a fair evaluation of the integration of this CO₂ capture process into a power plant process, an overall process evaluation is carried out. The use of detailed models of the power plant, of the compressor and of the CO₂ capture process enables the calculation of the power loss due to the steam extraction as well as due to the required auxiliary power for CO₂ compression, solvent and cooling pumps and mechanical chillers. To study the influence of the cold end of the process, two power plants with different cooling water temperatures are analysed. Additionally, two different process configurations of the capture plant, with either one single absorber or two absorbers connected in series where the first absorber captures the majority of the CO₂ and the second limits the NH₃ slip, are evaluated. The influence of the main process parameters (desorber pressure, solvent circulation rate, solvent recycling rate and chilling temperature) are evaluated and the optimal configuration with respect to the overall net efficiency penalty is determined. The study shows that the configuration of the process with absorption at low temperature (approximately 10°C) with or without precipitation of ammonium carbonate compounds leads to a lower net efficiency penalty than an MEA-based process, assuming that low temperature cooling water is available. An estimate of the size of the absorber shows that the absorber columns of an ammonia-based process are significantly higher than the ones required for an MEA-based process.

General information
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Main Research Area: Technical/natural sciences

Publication information
Evaluation of experimental data for wax and diamondoids solubility in gaseous systems

The Leveredge statistical approach is herein applied for evaluation of experimental data of the paraffin waxes/diamondoids solubility in gaseous systems. The calculation steps of this algorithm consist of determination of the statistical Hat matrix, sketching the Williams Plot, and calculation of the residuals of two selected correlations results. In addition, the applicability domains of the investigated correlations and quality of the existing experimental data are examined accompanied by outlier diagnostics. Two previously applied Chrastil-type correlations including the original Chrastil and Méndez-Santiago and Teja correlations are used to calculate/estimate the solubility of paraffin waxes (including n-C24H50 to n-C33H68) and diamondoids (adamantane and diamantane) in carbon dioxide/ethane gases, respectively. It can be interpreted from the obtained results that the applied equations for calculation of the corresponding solubilities are statistically valid and correct, and none of the experimental data can be designated as outliers.

General information

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Organisations: Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering, MINES ParisTech, Islamic Azad University

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Evaluation of data, Paraffin waxes, Diamondoids, Outlier diagnostics, Phase equilibrium data, Gaseous system

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Bibliographical note
Highlights:
- Leverage method is applied for evaluation of experimental phase equilibrium data.
- Solubility data of paraffin waxes/diamondoids in gaseous systems are studied.
- The Hat matrix, the Williams plot, and residuals are the elements of the method.
- The original Chrastil and Mèndez-Santiago and Teja correlations are used.
- It is interpreted that none of the experimental data can be designated as outliers

Experimental studies of low salinity water flooding in carbonate reservoirs: A new promising approach

Low salinity water flooding is well studied for sandstone reservoirs, both laboratory and field tests have showed improvement in the oil recovery in many cases. Up to very recently, the low salinity effect has been indeterminate for carbonates. Most recently, Saudi Aramco reported that substantial additional oil recovery can be achieved when successively flooding composite carbonate core plugs with various diluted versions of seawater. The experimental data on carbonates is very limited, so more data and better understanding of the mechanisms involved is needed to utilize this method for carbonate reservoirs. In this paper, we have experimentally investigated the oil recovery potential of low salinity water flooding for carbonate rocks. We used both reservoir carbonate and outcrop chalk core plugs. The flooding experiments were carried out initially with the seawater, and afterwards additional oil recovery was evaluated by sequential injection of various diluted seawater. The experiments applied stepwise increase in flow rate to eliminate the influence of possible capillary end effect. The total oil recovery, interaction of the different ions with the rock, and the wettability changes were studied both at ambient and high temperature. No low salinity effect was observed for the reservoir carbonate core plug at the ambient temperature, but increase of the pressure drop over the core plug was detected. On the contrary, a significant increase in oil recovery was observed under low salinity flooding of the reservoir carbonate core plugs at 90°C. An increase in pressure drop was also observed in this case, possibly related to migration of fines or dissolution reactions. The outcrop Aalborg chalk core plugs did not show any low salinity effect, both at the room and at a high temperature. In the light of experimental results, discussions are made about possible mechanisms for improving oil recovery in carbonate reservoir as a function of change in brine salinity. Copyright 2012, Society of Petroleum Engineers.

Experimental study and phase equilibrium modeling of systems containing acid gas and glycol

In this work, we study phase equilibria of systems containing acid gases and glycols. The acid gases include carbonyl sulfide (COS), hydrogen sulfide ($H_2S$), and carbon dioxide ($CO_2$), while glycols include monoethylene glycol (MEG), diethylene glycol (DEG), and triethylene glycol (TEG). A brief literature survey on the solubility of the acid gases and hydrocarbons in glycols is presented. New experimental solubility data mainly for COS and some limited data for $H_2S$ in
glycols from 276 to 333K and at elevated pressures are reported. Experimental measurements have been carried out using the "static-synthetic" method. The reliability and repeatability of the experimental work are demonstrated. The experimental solubility data for COS and glycols, from this work, and those for H₂S and CO₂ from the literature are modeled using the cubic-plus-association (CPA) equation of state (EoS). CPA parameters for pure components and binary systems are reported. Satisfactory correlations have been achieved using temperature-independent interaction parameters. Various modeling strategies and alternatives using CPA are tested and the results are critically evaluated. The variations and trends in the values of binary interaction parameters are discussed for the different systems studied.
Fast Nonconvex Model Predictive Control for Commercial Refrigeration

We consider the control of a commercial multi-zone refrigeration system, consisting of several cooling units that share a common compressor. The goal is to minimize the total energy cost, using real-time electricity prices, while obeying temperature constraints on the zones. We propose a variation on model predictive control to achieve this goal. When the right variables are used, the dynamics of the system are linear, and the constraints are convex. The cost function, however, is nonconvex. To handle this nonconvexity we propose a sequential convex optimization method, which typically converges in fewer than 5 or so iterations. We employ a fast convex quadratic programming solver to carry out the iterations, which is more than fast enough to run in real-time. We demonstrate our method on a realistic model, with a full year simulation, using real historical data. These simulations show substantial cost savings, and reveal how the method exhibits sophisticated response to real-time variations in electricity prices. This demand response is critical to help balance real-time uncertainties associated with large penetration of intermittent renewable energy sources in a future smart grid.

General information

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Fluid phase equilibria of the reaction mixture during the selective hydrogenation of 2-butenal in dense carbon dioxide

Knowledge of the phase behaviour and composition is of paramount importance for understanding multiphase reactions. We have investigated the effect of the phase behaviour in the palladium-catalysed selective hydrogenation of 2-butenal to saturated butanal in dense carbon dioxide. The reactions were performed using a 5wt% Pd on activated carbon in custom-designed high pressure autoclaves at 323K. The Cubic-Plus-Association (CPA) equation of state was employed to model the phase behaviour of the experimentally studied systems. CPA binary interaction parameters were estimated based on the experimental vapour–liquid or liquid–liquid equilibria data available in the literature. No experimental data for the CO2–2-butenal binary system were available in the literature; therefore, the bubble points of this mixture of varying composition at three different temperatures were measured in a high-pressure view cell. The results of the catalytic experiments showed that small amounts of carbon dioxide added to the system significantly decrease the conversion, whereas at higher loadings of CO2 the reaction rate gradually increases reaching a maximum. The CPA calculations revealed that this maximum is achieved in the so-called "expanded liquid" region, which is located near the critical point of the reacting mixture. It was also found that in this point the hydrogen concentration achieved its maximum in the CO2-expanded phase. Furthermore, the pressure – temperature regions where the multicomponent reaction system exists in one single phase and in multiphase were calculated.

General information
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Organisations: Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering, CHEC Research Centre, Swiss Federal Institute of Technology, Karlsruhe Institute of Technology KIT
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BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.303 SNIP 1.574 CiteScore 4.04
Web of Science (2014): Indexed yes
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Scopus rating (2013): SJR 1.426 SNIP 1.538 CiteScore 4.01
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Scopus rating (2012): SJR 1.549 SNIP 1.615 CiteScore 3.89
Framework for the analysis of crystallization operations

Crystallization is often applied in the production of salts and/or active pharmaceutical ingredients (API), and the crystallization step is an essential part of the manufacturing process for many chemicals-based products. In recent years the monitoring and analysis of crystallization operations has received increased attention due to the growing need to control more sophisticated production lines as well as to measure/monitor the final product characteristics. Crystallization operations involve a combination of several phenomena, and different kinetic models are required for their modeling. Growth of the crystals occurs in multiple dimensions and the relative rates of different growth and other kinetic phenomena control the shape and size distribution of the final product. Including several dimensions in the crystallization will allow a more general description of the kinetic phenomena and the crystallization operation. In order to have a full description of a crystallizer a combination of constitutive (kinetic) models is needed. Development of appropriate constitutive models requires data, which for size distributions in crystallization operations is available in the form of chord length distribution data (from Focused Beam Reflectance Measurements (FBRM)). Use of this data for modeling requires a data translation procedure.

The objective of this paper is to present a modeling procedure for systematic development of constitutive models for use in design, analysis and simulation of crystallization operations. This procedure has three main features: A data handling and translation feature, a constitutive model identification feature and a model application feature. For different crystallization operation scenarios, the measured data is translated to create an image of the product. Through the model identification option, the parameters of the constitutive models embedded within the crystallizer model are regressed to match the translated product image. With the models identified, they are applied to understand, design and/or analyze various crystallization operational scenarios.

The paper will present the constitutive model development procedure as part of a general crystallization modeling...
framework. It will highlight the different features through a case study involving measured data and use it to develop models and finally, the use of the model to analyze different crystallization operations.

**General information**

State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Center for Process Engineering and Technology, Center for Energy Resources Engineering, CERE – Center for Energy Resources Engineering
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Publication date: 2012
Event: Abstract from APACT-12, Newcastle, United Kingdom.
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Publication: Research › Conference abstract for conference – Annual report year: 2012

Fremstilling af dielektriske elektroaktive polymerer i stor skala

Interessen for dielektriske elektroaktive polymerfilm er de seneste år steget markant. For overhovedet at kunne producere de ønskede mængder til en konkurrencedygtig pris er optimering og effektivisering af produktionen af disse film et krav for teknologiens overlevelse.

**General information**

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Gravity Effect on Two-Phase Immiscible Flows in Communicating Layered Reservoirs

An upscaling method is developed for two-phase immiscible incompressible flows in layered reservoirs with good communication between the layers. It takes the effect of gravity into consideration. Waterflooding of petroleum reservoirs is used as a basic example for application of this method. An asymptotic analysis is applied to a system of 2D flow equations for incompressible fluids at high-anisotropy ratios, but low to moderate gravity ratios, which corresponds to the most often found reservoir conditions. The 2D Buckley–Leverett problem is reduced to a system of 1D parabolic equations in a layered reservoir. For low-gravity ratios, it can further be reduced to a system of hyperbolic equations. The number of the 1D equations in the system is equal to the number of layers in the reservoir. The method is tested on different examples of displacement in a layer-cake reservoir. Different combinations of gravity-viscous and anisotropy ratios are tested. Solutions by our method are compared with the results of 2D simulations carried out by the COMSOL solver. The results are comparable, especially if the layers of the reservoirs are further subdivided into sublayers, in order to account better for gravity segregation. The effects of gravity are analyzed.
High Order Adjoint Derivatives using ESDIRK Methods for Oil Reservoir Production Optimization

In production optimization, computation of the gradients is the computationally expensive step. We improve the computational efficiency of such algorithms by improving the gradient computation using high-order ESDIRK (Explicit Singly Diagonally Implicit Runge-Kutta) temporal integration methods and continuous adjoints. The high order integration scheme allows larger time steps and therefore faster solution times. We compare gradient computation by the continuous adjoint method to the discrete adjoint method and the finite-difference method. The methods are implemented for a two-phase flow reservoir simulator. Computational experiments demonstrate that the accuracy of the sensitivities obtained by the adjoint methods is comparable to the accuracy obtained by the finite difference method. The continuous adjoint method is able to use a different time grid than the forward integration. Therefore, it can compute these sensitivities much faster than the discrete adjoint method and the finite-difference method. On the other hand, the discrete adjoint method produces the gradients of the numerical schemes, which is beneficial for the numerical optimization algorithm. Computational experiments show that when the time steps are controlled in a certain range, the continuous adjoint method produces gradients sufficiently accurate for the optimization algorithm and somewhat faster than the discrete adjoint method.

General information
State: Published
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History Matching: Towards Geologically Reasonable Models
This work focuses on the development of a new method for history matching problem that through a deterministic search finds a geologically feasible solution. Complex geology is taken into account evaluating multiple point statistics from earth model prototypes - training images. Further a function that measures similarity between statistics of a training image and statistics of any smooth model is introduced and its analytical gradient is computed. This allows us to apply any gradient-based method to history matching problem and guide a solution until it satisfies both production data and complexity of a prior model with desired accuracy. As a consequence of the approach, we sufficiently decrease the amount of forward simulations needed to resolve historical data and prior information.

General information
State: Published
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Number of pages: 5
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Main Research Area: Technical/natural sciences
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Melnikova et al., 2012 - Extended abstract EAGE Dubai.pdf
Improving multiple-point-based a priori models for inverse problems by combining Sequential Simulation with the Frequency Matching Method

In order to move beyond simplified covariance based a priori models, which are typically used for inverse problems, more complex multiple-point-based a priori models have to be considered. By means of marginal probability distributions 'learned' from a training image, sequential simulation has proven to be an efficient way of obtaining multiple realizations that honor the same multiple-point statistics as the training image. The frequency matching method provides an alternative way of formulating multiple-point-based a priori models. In this strategy the pattern frequency distributions (i.e. marginals) of the training image and a subsurface model are matched in order to obtain a solution with the same multiple-point statistics as the training image. Sequential Gibbs sampling is a simulation strategy that provides an efficient way of applying sequential simulation based algorithms as a priori information in probabilistic inverse problems. Unfortunately, when this strategy is applied with the multiple-point-based simulation algorithm SNESIM the reproducibility of training image patterns is violated. In this study we suggest to combine sequential simulation with the frequency matching method in order to improve the pattern reproducibility while maintaining the efficiency of the sequential Gibbs sampling strategy. We compare realizations of three types of a priori models. Finally, the results are exemplified through crosshole travel time tomography.

Influence of effective stress coefficient on mechanical failure of chalk

The Effective stress coefficient is a measure of how chalk grains are connected with each other. The stiffness of chalk may decrease if the amount of contact cements between the grains decreases, which may lead to an increase of the effective stress coefficient. We performed CO2 injection in chalk, as this process could affect the grain contact cement. If this happens, the effective stress at the grain contacts in a reservoir will change according to the effective stress principle of Biot. In a $p'$-$q$ space for failure analysis, we observed that a higher effective stress coefficient reduces the elastic region and vice versa. However, as the effective stress working on the rock decreases with increased effective stress coefficient, the reduction of elastic region will have less effect on pore collapse strength if we consider the change in the effective stress coefficient. This finding will help estimate a more precise failure strength of chalk during changed stress state and under the influence of chemically reactive fluids during production of hydrocarbon and geological storage CO2.
Iterative Methods for MPC on Graphical Processing Units

The high floating point performance and memory bandwidth of Graphical Processing Units (GPUs) makes them ideal for a large number of computations which often arises in scientific computing, such as matrix operations. GPUs achieve this performance by utilizing massive parallelism, which requires reevaluating existing algorithms with respect to this new architecture. This is of particular interest to large-scale constrained optimization problems with real-time requirements. The aim of this study is to investigate different methods for solving large-scale optimization problems with focus on their applicability for GPUs. We examine published techniques for iterative methods in interior points methods (IPMs) by applying them to simple test cases, such as a system of masses connected by springs. Iterative methods allow us deal with the ill-conditioning occurring in the later iterations of the IPM as well as to avoid the use of dense matrices, which may be too large for the limited memory capacity of current graphics cards.

General information
State: Published
Organizations: Center for Energy Resources Engineering, Scientific Computing, Department of Informatics and Mathematical Modeling
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Pages: 161
Publication date: 2012

Kinetics of absorption of carbon dioxide into aqueous potassium salt of proline

The absorption of carbon dioxide (CO₂) into aqueous solution of potassium prolinate (KPr) are studied at 303, 313, and 323K within the salt concentration range of 0.5–3.0kmolm⁻³ using a wetted wall column absorber. The experimental results are used to interpret the kinetics of the reaction of CO₂ with KPr for the above mentioned concentration and temperature range. Following the reaction mechanism of CO₂ with primary and secondary alkanolamines, the reaction of CO₂ with KPr is also described using zwitterionic mechanism. Based on the pseudo-first-order condition for the CO₂ absorption, the reaction rate parameters are determined from the kinetic measurements and presented at each experimental condition. The reaction order is found to be in between 1.36 and 1.40 with respect to KPr for the above mentioned concentration range. The second-order rate constants, k₂, are obtained as 118,914, 203,851, and 317,625m³kmol⁻¹s⁻¹ at 303, 313, and 323K, respectively with activation energy of 36.5kJmol⁻¹. The second-order rate constants are much higher than for alkanolamines and some other salt of amino acids.

General information
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Organizations: Center for Energy Resources Engineering, CERE – Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering
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Limits to Nonlinear Inversion

For non-linear inverse problems, the mathematical structure of the mapping from model parameters to data is usually unknown or partly unknown. Absence of information about the mathematical structure of this function prevents us from presenting an analytical solution, so our solution depends on our ability to produce efficient search algorithms. Such algorithms may be completely problem-independent (which is the case for the so-called 'meta-heuristics' or 'blind-search' algorithms), or they may be designed with the structure of the concrete problem in mind. We show that pure meta-heuristics are inefficient for large-scale, non-linear inverse problems, and that the 'no-free-lunch' theorem holds. We discuss typical objections to the relevance of this theorem. A consequence of the no-free-lunch theorem is that algorithms adapted to the mathematical structure of the problem perform more efficiently than pure meta-heuristics. We study problem-adapted inversion algorithms that exploit the knowledge of the smoothness of the misfit function of the problem. Optimal sampling strategies exist for such problems, but many of these problems remain hard. © 2012 Springer-Verlag.
Managing Injected Water Composition To Improve Oil Recovery: A Case Study of North Sea Chalk Reservoirs

In recent years, many core displacement experiments of oil by seawater performed on chalk rock samples have reported \( \text{SO}_4^{2-} \), \( \text{Ca}^{2+} \), and \( \text{Mg}^{2+} \) as potential determining ions for improving oil recovery. Most of these studies were carried out with outcrop chalk core plugs. The objective of this study is to investigate the potential of the advanced waterflooding process by carrying out experiments with reservoir chalk samples. The study results in a better understanding of the mechanisms involved in increasing the oil recovery with potential determining ions. We carried out waterflooding instead of spontaneous imbibition, which has been applied in most of the previous studies. Two different flooding schemes (with and without aging) were used for flooding North Sea reservoir chalk samples. For comparison, two tests were also carried out with Stevns Klint core plugs. The flooding tests were carried out with the following injecting fluids: distilled water, brine with and without sulfate, and brine containing only magnesium ions. The total oil recovery, recovery rate, and interaction mechanisms of ions with rock were studied for different injecting fluids at different temperatures and wettability conditions. Studies of the temperature dependence of the oil recovery indicated that the interaction of the ions contained in brine with the rock cannot be the only determining mechanism of enhanced recovery. We observed no substitution of \( \text{Ca}^{2+} \) ions with \( \text{Mg}^{2+} \) ions at high temperatures for both rocks. Not only the injection brine composition but also the formation water composition affected the oil recovery at high temperatures from the Stevns Klint chalk rock.

General information

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Organisations: Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering, Department of Chemistry
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Scopus rating (2013): CiteScore 3.52
Measurement and Modelling of the Piperazine Potassium Carbonate Solutions for CO2 Capture

The climate is in a critical state due to the impact of pollution by CO2 and similar greenhouse gases. Action needs to be taken in order reduce the emission of harmful components. CO2 capture is one process to help the world population back on track in order to return to normal condition, obtaining a sustainable use of natural organic resources. In this work the solid solubility has been measured for the promoted hot carbonate process using piperazine and K2CO3/KHCO3. It entails a comparison of several newly developed methods in order to guarantee the accuracy of determined experimental work. Interesting and difficult phenomena has been observed in the analysis of the piperazine solvent. Various hydrates and complexes are formed. The loaded solutions are analysed using the same techniques. Guidelines for solvent handling are set up. These define a simple boundary for safe solvent handling in order to prevent precipitation during mixing. At the same time these can actively be used in the development in the process. Slurry formation is a core issue in these processes and need to be addressed carefully. The outcome of thermodynamic modelling by using the extended UNIQUAC model will be shown with the purpose of simulating the CO2 capture process. This involves equilibrium studies on physical properties in the activated carbonate solvent. Energy consumption while applying the promoted carbonate solutions using piperazine is given in overview.
Modeling Operating Modes during Plant Life Cycle

Modelling process plants during normal operation requires a set of basic assumptions to define the desired functionalities which lead to fulfillment of the operational goal(s) for the plant. However, during start-up and shut down as well as during batch operation an ensemble of interrelated modes are required to cover the whole operational window of a process plant including intermediary operating modes. Development of such an ensemble for a plant would constitute a systematic way of defining the possible plant operating modes and thus provide a platform for also defining a set of candidate control structures. The present contribution focuses on development of a model ensemble for a plant with an illustrative example for a bioreactor.

Starting from a functional model a process plant may be conceptually designed and qualitative operating models may be developed to cover the different regions within the plant operating window, including transitions between operating regions. Subsequently qualitative functional models may be developed when the means for achieving the desired functionality are sufficiently specified during the design process. Quantitative mathematical models of plant physics can be used for detailed design and optimization. However, the qualitative functional models already provide a systematic framework based on the notion of means-end abstraction hierarchies. Thereby, functional modeling provides a scientific basis for managing complexity. A functional modelling framework has been implemented to facilitate model development and application in a computer environment. Defining means-end causal relations makes it possible to perform qualitative causal reasoning within a functional modelling framework. Thus such a framework renders it possible to develop potentially feasible control structures. This ability is based on goal reasoning and development of goal trees from causal relations. These capabilities of functional models extend the application potential of functional modelling significantly beyond that of conventional mathematical modeling representing quantitative physical phenomena. The example case is a continuously operating bioreactor for manufacturing single cell protein from methane where also the bioreactor start-up is illustrated with switching between operating modes and their associated control structures as seen in a multiloop control configuration.

General information

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Organisations: Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Department of Electrical Engineering, Automation and Control
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Modeling Smart Energy Systems for Model Predictive Control

Integrating large amounts of renewable energy sources like wind and solar power introduces large fluctuations in the power production. Either this energy must be stored or consumed right away. Storage solutions are very expensive and not applicable everywhere. So utilizing all of this green energy as it is produced requires a very flexible and controllable power consumption. Examples of controllable electric loads are heat pumps in buildings and Electric Vehicles (EVs) that are expected to play a large role in the future Danish energy system. These units in a smart energy system can potentially offer flexibility on a time scale ranging from seconds to several days by moving power consumption, exploiting thermal inertia or battery storage capacity, respectively. Using advanced control algorithms these systems are able to reduce their own electricity costs by planning ahead and moving consumption to periods with green and cheap electricity. This situation
occurs when there is a lot of excess wind power in the system which is reflected in the electricity price and in turn creates an incentive to absorb the energy. In this paper a decentralized control strategy is investigated where prices indirectly influence the total power consumption of the smart energy systems connected to the power grid. Compared to a direct control strategy the complexity of the problem is reduced and decreases both the computation efforts and the need for communication. However, not only the current price, but a forecast of the expected future price should also be available in order for the individual units to plan ahead in the most feasible way. This is necessary since Economic MPCs do not respond to the absolute cost of electricity, but to variations of the price over the prediction horizon. Economic MPC is ideal for price responsive units where the model is known very well. Constraints and disturbance forecasts are straightforward to implement in the controller. MPC relies on the receding horizon principle, where a new optimal control signal is calculated at each time step for the prediction horizon. Only the optimal control signal at the current time step is implemented and consequently closed loop feedback is obtained. A generic model of an energy component is proposed in this paper, so the same Economic MPC framework can be used to design controllers for the different units. However, different signals and forecast, e.g. weather forecasts and usage patterns, are used depending on the unit. The generic state space will be a discrete time state space model with hard input constraints and soft output constraints. For the considered energy systems there is usually a strict limit on the maximum available power, but the output, e.g. a temperature or an EV battery state of charge, can often be relaxed. The output constraints thus define a band of operation, that can be time varying, and the controller must keep the output within these limits in the cheapest possible way. In this paper the price forecast available by all units is assumed to be known and equal to the day-ahead elspot price from the Nordic electricity exchange market NordPool. The resulting electricity cost savings compared to an MPC with no price considerations are around 30-50% for the chosen units. In future work the price could be replaced by an intrahour price that is related to the deviation between the planned and the actual consumption. In this way all units are motivated to stick to the predicted consumption plan.

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Model Predictive Control Algorithms for Pen and Pump Insulin Administration
Despite recent developments within diabetes management such as rapid-acting insulin, continuous glucose monitors (CGM) and insulin pumps, tight blood glucose control still remains a challenge. A fully automated closed-loop controller, also known as an artificial pancreas (AP), has the potential to ease the life and reduce the risk of acute and chronic diabetic complications. However, the noise associated to CGMs, the long insulin action time for continuous subcutaneous infusion of insulin (CSII) pumps, and the high intra- and inter-patient variability significantly limits the performance of current closed-loop controllers.

In this thesis, we present different control strategies based on Model Predictive Control (MPC) for an artificial pancreas. We use Nonlinear Model Predictive Control (NMPC) in order to determine the optimal insulin and blood glucose profiles. The optimal control problem (OCP) is solved using a multiple-shooting based algorithm. We use an explicit Runge-Kutta method (DOPRI45) with an adaptive stepsize for numerical integration and sensitivity computation. The OCP is solved using a Quasi-Newton sequential quadratic programming (SQP) with a linesearch and a BFGS update for the Hessian of the Lagrangian. In addition, we apply a Continuous-Discrete Extended Kalman Filter (CDEKF) in order to simulate cases where the meal size is uncertain, or even unannounced.

We also propose a novel control strategy based on linear MPC for overnight stabilization of blood glucose. The model parameters are personalized using a priori available patient information. We consider an autoregressive integrated moving
average with exogenous input (ARIMAX) model. We summarize and the results of the overnight clinical studies conducted at Hvidovre Hospital. Based on these results, we propose improvements for the stochastic part of our controller model. We state and compare three different stochastic model structures. The first one is the ARIMAX structure that has been used for the clinical studies. The second one is an autoregressive moving average with exogenous input (ARMAX) model. The third one is an adaptive ARMAX model in which we estimate the parameters of the stochastic part using a Recursive Least Square (RLS) method. We test the controller in a virtual clinic of 100 patients. This virtual clinic is based on the Hovorka model. We consider the case where only half of the bolus is administrated at mealtime, and the case where the insulin sensitivity increases during the night.

This thesis consists of a summary report, glucose and insulin profiles of the clinical studies and research papers submitted, peer-reviewed and/or published in the period September 2009 - September 2012.

General information
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Model Predictive Control for an Industrial SAG Mill
We discuss Model Predictive Control (MPC) based on ARX models and a simple lower order disturbance model. The advantage of this MPC formulation is that it has few tuning parameters and is based on an ARX prediction model that can readily be identified using standard technologies from system identification. When applied to MIMO systems we call this controller a MIMO-ARX based MPC. We use an industrial Semi-Autogenous Grinding (SAG) mill to illustrate the performance of this controller. SAG mills are the primary units in a grinding chain and also the most power consuming units. Therefore, improved control of SAG mills has the potential to significantly improve efficiency and reduce the specific energy consumption for mineral processes. Grinding circuits involving SAG mills are multivariate processes. Commissioning of a control system based on a classical single-loop controllers with logic is time consuming, while MPC has the potential to both improve the control performance and the commissioning time and expertise required. The simulation results demonstrate that the MPC based on a MIMO-ARX model is able to provide nice control performance measured by its ability to track an output reference and reject unknown disturbances. Furthermore, the method used to design the controller represents a systematic method that can be automatized for wide-spread deployment in industrial environments.

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Pages: 208
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Model predictive control for a smart solar tank based on weather and consumption forecasts

In this work the heat dynamics of a storage tank were modelled on the basis of data and maximum likelihood methods. The resulting grey-box model was used for Economic Model Predictive Control (MPC) of the energy in the tank. The control objective was to balance the energy from a solar collector and the heat consumption in a residential house. The storage tank provides heat in periods where there is low solar radiation and stores heat when there is surplus solar heat. The forecasts of consumption patterns were based on data obtained from meters in a group of single-family houses in Denmark. The tank can also be heated by electric heating elements if necessary, but the electricity costs of operating these heating elements should be minimized. Consequently, the heating elements should be used in periods with cheap electricity. It is proposed to integrate a price-sensitive control to enable the storage tank to serve a smart energy system in which flexible consumers are expected to help balance fluctuating renewable energy sources like wind and solar. Through simulations, the impact of applying Economic MPC shows annual electricity cost savings up to 25-30%.
Model predictive control technologies for efficient and flexible power consumption in refrigeration systems

Considerable amounts of energy are consumed in supermarket refrigeration systems worldwide. Due to the thermal capacity of refrigerated goods and the rather simplistic control most commonly applied, there is a potential for distributing the system load over time in a more cost-optimal way. In this paper we describe a novel economic-optimizing Model Predictive Control (MPC) scheme that reduces operating costs by utilizing the thermal storage capabilities. A nonlinear optimization tool to handle a non-convex cost function is utilized for simulations with validated scenarios. In this way we explicitly address advantages from daily variations in outdoor temperature and electricity prices. Secondly, we formulate a new cost function that enables the refrigeration system to contribute with ancillary services to the balancing power market. This involvement can be economically beneficial for the system itself, while crucial services can be delivered to a future flexible and intelligent power grid (Smart Grid). Furthermore, we discuss a novel incorporation of probabilistic constraints and Second Order Cone Programming (SOCP) with economic MPC. A Finite Impulse Response (FIR) formulation of the system models allows us to describe and handle model as well as prediction uncertainties in this framework. This means we can demonstrate means for robustifying the performance of the controller.
Monte Carlo full-waveform inversion of crosshole GPR data using multiple-point geostatistical a priori information
We present a general Monte Carlo full-waveform inversion strategy that integrates a priori information described by geostatistical algorithms with Bayesian inverse problem theory. The extended Metropolis algorithm can be used to sample the a posteriori probability density of highly nonlinear inverse problems, such as full-waveform inversion. Sequential Gibbs sampling is a method that allows efficient sampling of a priori probability densities described by geostatistical algorithms based on either two-point (e.g., Gaussian) or multiple-point statistics. We outline the theoretical framework for a full-waveform inversion strategy that integrates the extended Metropolis algorithm with sequential Gibbs sampling such that arbitrary complex geostatistically defined a priori information can be included. At the same time we show how temporally and/or spatially correlated data uncertainties can be taken into account during the inversion. The suggested inversion strategy is tested on synthetic tomographic crosshole ground-penetrating radar full-waveform data using multiple-point-based a priori information. This is, to our knowledge, the first example of obtaining a posteriori realizations of a full-waveform inverse problem. Benefits of the proposed methodology compared with deterministic inversion approaches include: (1) The a posteriori model variability reflects the states of information provided by the data uncertainties and a priori information, which provides a means of obtaining resolution analysis. (2) Based on a posteriori realizations, complicated statistical questions can be answered, such as the probability of connectivity across a layer. (3) Complex a priori information can be included through geostatistical algorithms. These benefits, however, require more computing resources than traditional methods do. Moreover, an adequate knowledge of data uncertainties and a priori information is required to obtain meaningful uncertainty estimates. The latter may be a key challenge when considering field experiments, which will not be addressed here.

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MPC Toolbox with GPU Accelerated Optimization Algorithms
The introduction of Graphical Processing Units (GPUs) in scientific computing has shown great promise in many different fields. While GPUs are capable of very high floating point performance and memory bandwidth, its massively parallel architecture requires algorithms to be reimplemented to suit the different architecture. Interior point method can be used to solve convex optimization problems. These problems often arise in fields such as in Model Predictive Control (MPC), which may have real-time requirements for the solution time. This paper presents a case study in which we utilize GPUs for a Linear Programming Interior Point Method to solve a test case where a series of power plants must be controlled to minimize the cost of power production. We demonstrate that using GPUs for solving MPC problems can provide a speedup in solution time.

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Novel self-associative and multiphase nanostructured soft carriers based on amphiphilic hyaluronic acid derivatives
The purpose of the present study was to investigate the physicochemical properties in aqueous media of amphiphilic hyaluronic acid (HA) derivatives obtained by reaction of HA’s hydroxyl groups with octenyl succinic anhydride (OSA). The self-associative properties of the resulting octenyl succinic anhydridemodified hyaluronic acid (OSA-HA) derivatives were studied by fluorescence spectroscopy using Nile Red as fluorophore. The morphology, size and surface charge of the OSA-HA assemblies were determined by transmission electron microscopy, dynamic light scattering and by measuring their electrophoretic mobility, respectively. OSA-HA was shown to spontaneously self-associate in aqueous media into negatively charged spherical and multiphasic nanostructures with a hydrodynamic diameter between 170 and 230 nm and to solubilize hydrophobic compounds such as Nile Red. This was a good indication that OSAHA could be used as building block for the formulation of soft nanocarriers towards the encapsulation and controlled delivery of hydrophobic active ingredients or drugs.

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Organisations: Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Ressources Engineering, University of Geneva, Novozymes A/S
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Novel silicone compatible cross-linkers for controlled and well distributed functionalization of PDMS networks

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Organisations: Department of Chemical and Biochemical Engineering, The Danish Polymer Centre, Center for Energy Resources Engineering
Numerical Methods for Solution of the Extended Linear Quadratic Control Problem
In this paper we present the extended linear quadratic control problem, its efficient solution, and a discussion of how it arises in the numerical solution of nonlinear model predictive control problems. The extended linear quadratic control problem is the optimal control problem corresponding to the Karush-Kuhn-Tucker system that constitute the majority of computational work in constrained nonlinear and linear model predictive control problems solved by efficient MPC-tailored interior-point and active-set algorithms. We state various methods of solving the extended linear quadratic control problem and discuss instances in which it arises. The methods discussed in the paper have been implemented in efficient C code for both CPUs and GPUs for a number of test examples.

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Oil Reservoir Production Optimization using Single Shooting and ESDIRK Methods
Conventional recovery techniques enable recovery of 10-50% of the oil in an oil field. Advances in smart well technology and enhanced oil recovery techniques enable significant larger recovery. To realize this potential, feedback model-based optimal control technologies are needed to manipulate the injections and oil production such that flow is uniform in a given geological structure. Even in the case of conventional water flooding, feedback based optimal control technologies may enable higher oil recovery than with conventional operational strategies. The optimal control problems that must be solved are large-scale problems and require specialized numerical algorithms. In this paper, we combine a single shooting optimization algorithm based on sequential quadratic programming (SQP) with explicit singly diagonally implicit Runge-Kutta (ESDIRK) integration methods and the a continuous adjoint method for sensitivity computation. We demonstrate the procedure on a waterflooding example with conventional injectors and producers.

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On multiphase negative flash for ideal solutions

There is a recent interest to solve multiphase negative flash problems where the phase amounts can be negative for normal positive feed composition. Solving such a negative flash problem using successive substitution needs an inner loop for phase distribution calculation at constant fugacity coefficients. It is shown that this inner loop, named here as multiphase negative flash for ideal solutions, can be solved either by Michelsen's algorithm for multiphase normal flash, or by its variation which uses F−1 phase amounts as independent variables. In either case, the resulting algorithm is actually simpler than the corresponding normal flash algorithm. Unlike normal flash, multiphase negative flash for ideal solutions can diverge if the feasible domain for phase amounts is not closed. This can be judged readily during the iteration process. The algorithm can also be extended to the partial negative flash situation where several phase amounts must be non-negative and at least one phase amount can be negative.
Optimal Energy Consumption in Refrigeration Systems - Modelling and Non-Convex Optimisation

Supermarket refrigeration consumes substantial amounts of energy. However, due to the thermal capacity of the refrigerated goods, parts of the cooling capacity delivered can be shifted in time without deteriorating the food quality. In this study, we develop a realistic model for the energy consumption in supermarket refrigeration systems. This model is used in a Nonlinear Model Predictive Controller (NMPC) to minimise the energy used by operation of a supermarket refrigeration system. The model is non-convex and we develop a computational efficient algorithm tailored to this problem that is somewhat more efficient than general purpose optimisation algorithms for NMPC and still near to optimal. Since the non-convex cost function has multiple extrema, standard methods for optimisation cannot be directly applied. A qualitative analysis of the system's constraints is presented and a unique minimum within the feasible region is identified. Following that finding we propose a tailored minimisation procedure that utilises the nature of the feasible region such that the minimisation can be separated into two linear programs; one for each of the control variables. These subproblems are simple to solve but some iterations might have to be performed in order to comply with the maximum capacity constraint. Finally, a nonlinear solver is used for a small example without separating the optimisation problem, and the results are compared to the outcome of our proposed minimisation procedure for the same conceptual example. The tailored approach is somewhat faster than the general optimisation method and the solutions obtained are almost identical.

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Organisations: Center for Energy Resources Engineering, Scientific Computing, Department of Informatics and Mathematical Modeling, Danfoss A/S, Institute for Product Development
Optimisation of Oil Production in Two – Phase Flow Reservoir Using Simultaneous Method and Interior Point Optimiser

Natural petroleum reservoirs are characterised by 2-phase flow of oil and water in the porous media (e.g. rocks) which they are built of. Conventional methods of extracting oil from those fields, which utilise high initial pressure obtained from
natural drive, leave more than 70% of oil in the reservoir. A promising decrease of these remained resources can be provided by smart wells applying water injections to sustain satisfactory pressure level in the reservoir throughout the whole process of oil production. Basically to enhance secondary recovery of the remaining oil after drilling, water is injected at the injection wells of the down-hole pipes. This sustains the pressure in the reservoir and drives oil towards production wells. There are however, many factors contributing to the poor conventional secondary recovery methods e.g. strong surface tension, heterogeneity of the porous rock structure leading to change of permeability with position in the reservoir, or high oil viscosity. Therefore it is desired to take into account all these phenomena by implementing a realistic simulator of the 2-phase flow reservoir, which imposes the set of constraints on the state variables of optimisation problem. Then, thanks to optimal control, it is possible to adjust effectively injection valves to control 2 phase immiscible flow in every grid block of the reservoir and navigate oil to the production wells so it does not remain in the porous media. The use of such a smart technology known also as smart fields, or closed loop optimisation, can be used for optimising the reservoir performance in terms of net present value of oil recovery or another economic objective. In order to solve an optimal control problem we use a direct collocation method where we translate a continuous problem into a discrete one by applying explicit and implicit Euler methods. A substantial challenge of finding optimal solution in a robust way comes along with handling the scale of the optimal control problem due to discretisation in time and space. Consequently, an Ipopt (Interior Point Optimiser) open source software for large scale nonlinear optimisation was applied. Because of its versatile compatibility with programming technologies, a C++ programming language in Microsoft Visual Studio integrated development environment was used for modelling the optimal control problem. Thanks to object oriented features of the language, it was possible to approach the problem in a very modular way by automating the discretisation process and develop interfaces for retrieving information from a continuous problem. When tackling this problem, we reduce approximation error made by discretising of the original problem, by increasing the number of simulation steps and therefore it is necessary to solve large instances of the reformulation. As a result, it is very suitable to use Ipopt algorithm which implements an interior-point linesearch filter method making it very powerful for solving large problems with up to hundreds of millions of constraints and variables.

**Optimization based tuning approach for offset free MPC**

We present an optimization based tuning procedure with certain robustness properties for an offset free Model Predictive Controller (MPC). The MPC is designed for multivariate processes that can be represented by an ARX model. The advantage of ARX model representations is that standard system identification techniques using convex optimization can be used for identification of such models from input-output data. The stochastic model of the ARX model identified from input-output data is modified with an ARMA model designed as part of the MPC-design procedure to ensure offset-free control. The ARMAX model description resulting from the extension can be realized as a state space model in innovation form. The MPC is designed and implemented based on this state space model in innovation form. Expressions for the closed-loop dynamics of the unconstrained system is used to derive the sensitivity function of this system. The closed-loop expressions are also used to numerically evaluate absolute integral performance measures. Due to the closed-loop evaluations these evaluations can be done relative quickly. Consequently, the tuning may be performed by numerical minimization of the integrated absolute error subject to a constraint on the maximum of the sensitivity function. The latter constraint provides a robustness measure that is essential for the procedure. The method is demonstrated on two simulated examples: A Wood-Berry distillation column example and a cement mill example.
 Overnight Control of Blood Glucose in People with Type 1 Diabetes

In this paper, we develop and test a Model Predictive Controller (MPC) for overnight stabilization of blood glucose in people with type 1 diabetes. The controller uses glucose measurements from a continuous glucose monitor (CGM) and its decisions are implemented by a continuous subcutaneous insulin infusion (CSII) pump. Based on a priori patient information, we propose a systematic method for computation of the model parameters in the MPC. Safety layers improve the controller robustness and reduce the risk of hypoglycemia. The controller is evaluated in silico on a cohort of 100 randomly generated patients with a representative intersubject variability. This cohort is simulated overnight with realistic variations in the insulin sensitivities and needs. Finally, we provide results for the first tests of this controller in a real clinic.

Particles in Pores: Stochastic Modeling of Polydisperse Transport

Colloid flow, filtration, and migration in porous media are widely observed in important natural and industrial processes, such as pathogen (bacteria) spreading in aquifers, colloid-facilitated migration of heavy metal in soils, mud filtration during drilling wells, injectivity decline during water injection, and deep bed filtration during waste water treatment. The current thesis aims at better understanding the transport and fate of colloids in porous media. A number of methodologies have been applied in this study, such as developing new mathematical models for colloid filtration, comparing the modeling results to experimental observations, uncertainty and sensitivity analysis of the new models, and realizing the pore-scale physics in network models.

This thesis has been compiled in such a way that each chapter arises from a self-contained study targeting a particular
problem of colloid filtration: (1) Recent advances in colloids filtration theory; (2) Non-Fickian Transport and heterogeneous attachment of colloids; (3) Uncertainty and sensitivity analysis of models for non-Fickian transport and heterogeneous attachment; (4) Prediction of injectivity decline during waterflooding; (5) Colloid migration and recapture; (6) Induced colloid migration for enhanced oil recovery; (7) Estimating filtration coefficients for straining.

These studies have been separately published as journal papers, conference papers and book chapters. Nevertheless, they are not independent of one another but logically connected. The connections and main findings can be summarized as follows:

1. The discrepancies between the classical colloid filtration theory and experimental observations have been overviewed in Chapter 1. Many of them are observed under unfavorable attachment conditions, such as hyperexponential and non-monotonic deposition profiles. Such behavior of colloids is attributed to the heterogeneous attachment (Chapters 2 and 3) and the migration of colloids (Chapter 5), respectively.
2. A second reason for the deposition hyperexponentiality is the non-Fickian transport due to the heterogeneity of porous media. It also explains the dispersed and asymmetrical breakthrough curves of tracers in natural porous media (Chapters 2 and 3). Chapter 2 shows that the elliptic equation can be applied to capture the non-Fickian behaviors of colloids and tracers in porous media. It is closely followed by Chapter 3, the uncertainty and sensitivity analysis of the model predictions and the parameter estimation. Suggestions for experimental design for accurate determination of the model parameters are also provided.
3. Chapters 2 and 3 form a thorough study of the integral model for colloid filtration with non-Fickian transport and heterogeneous attachment. They are followed by the study of applying of such a model in the petroleum industry to predict injectivity decline during waterflooding in Chapter 4. However, the non-Fickian behavior of particles around the injection well is shown not to be significant. The reasons are that the temporal dispersion term is inverse proportional to the particle velocity and that the particle velocity is higher close to the well than that far away from the well.
4. The criterion of an attached colloid particle to be re-entrained by the hydrodynamic drag into the bulk fluid is the torques of detachment exceeding those of attachment. Bearing such a criterion in mind, the erosion of external cake, the migration of surface-associated colloids during one phase flow, and the migration of reservoir fines during two-phase flow are studied in similar fashions (Chapters 4, 5, 6). The erosion of external cakes in the injection wells gives rise to the steady stage of the injectivity and filling rat holes in the well (Chapter 4). The migration of surface-associated colloids gives rise to non-monotonic deposition profiles (Chapter 5). Migration and straining of reservoir fines may enhance oil recovery by increasing the sweep efficiency (Chapter 6).
5. Another important mechanism for particle capture is straining or size exclusion of colloids. Such phenomena are closely tied to the migration of colloids under unfavorable attachment conditions: surface-associated colloids rolling to straining sites (grain-grain contacts, pore throats) in Chapter 5, and the straining of released reservoir fines at pore throats in Chapter 6. However, the straining mechanism is described by nothing more than a straining rate coefficient in these studies. Finally in Chapter 7, a much better understanding of straining is achieved by the study of pore scale physics in a network model. The filtration coefficient for straining is estimated from the particle size and the pore size distributions. A new capture scheme of straining (minimum capture) is proposed to explain the large penetration depths of colloids in porous media and the power law dependencies of filtration coefficients in the experiments.

General information
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Phase Equilibria of Three Binary Mixtures: Methanethiol + Methane, Methanethiol + Nitrogen, and Methanethiol + Carbon Dioxide

New vapor–liquid equilibrium (VLE) data for methanethiol (MM) + methane (CH₄), methanethiol (MM) + nitrogen (N₂), and methanethiol (MM) + carbon dioxide (CO₂) is reported for temperatures of (304, 334, and 364) K in the pressure range (1 to 8) MPa. A “static–analytic” method was used for performing the measurements. The objective is to provide experimental VLE data for methanethiol with other natural gas contents at its crude form, for which no data are available in the open literature. The new VLE data for the aforementioned systems have been modeled successfully with the cubic-plus-association equation of state (CPA EoS).

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Phase equilibrium modeling of gas hydrate systems for CO₂ capture

Two thermodynamic models capable of describing dissociation pressures of mixed gas clathrate hydrates formed from ternary mixtures of CO₂, N₂, and liquid water, are presented. Both of the models utilize the Cubic-Plus-Association (CPA) equation of state (EOS) for the thermodynamic description of the non-solid phases (vapor and liquid). The solid hydrate phase is described by the van der Waals–Platteeuw model as presented by Parrish and Prausnitz. An algorithm for combining the CPA EOS with the van der Waals–Platteeuw model in a calculation of hydrate dissociation pressure is presented. Two models are described in this work. They differ in their method for describing the Langmuir adsorption coefficients in the van der Waals–Platteeuw model. These models are named Model I and Model II. Model I utilizes a statistical thermodynamics approach based on Lennard-Jones–Devonshire theory, using the spherical core Kihara cell potential. Model II uses a two-parameter explicit expression for the Langmuir adsorption coefficient, based on Langmuir adsorption theory. With two hydrate formers, four parameters in the Kihara cell potentials are fitted for Model I. Sixteen parameters are required to be fitted for Model II. The two model parameter sets are fitted to pure hydrate dissociation pressures and mixed hydrate dissociation pressures found in literature. In the fitting process, vapor phases with initial mole fractions of CO₂ below 0.15 are assumed to form structure II hydrates, while structure I hydrates are assumed to form from vapor phases with initial mole fractions of CO₂ at or above 0.15. The two models are validated against mixed hydrate equilibrium data found in literature. Both dissociation pressures and hydrate compositions are considered in the validation process. With the fitted parameters, Model I predicts a hydrate structure transition from structure II hydrates at vapor phase mole fractions of CO₂ below 0.12 to 0.15 (depending on temperature) to structure I hydrates at mole fractions of CO₂ above this concentration range. The exact transition concentration is shown to increase with increasing temperature. Model II predicts structure I hydrates to be stable in concentrations down to vapor phase mole fractions of CO₂ in the order of 0.001 to 0.02, depending on temperature. Model II predicts the transition concentration to decrease with increasing temperature. Since there is disparity amongst the different literature data for this system, it was not possible to determine unequivocally, which of the two models perform better.
Pore Radius and Permeability Prediction from Sonic Velocity

General information
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Organisations: Department of Civil Engineering, Section for Geotechnics and Geology, Center for Energy Resources Engineering

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Process simulation of CO$_2$ capture with aqueous ammonia using the Extended UNIQUAC model

The use of aqueous ammonia is a promising option to capture carbon dioxide from power plants thanks to the potential low heat requirement during the carbon dioxide desorption compared to monoethanolamine (MEA) based process. The patented Chilled Ammonia Process developed by Alstom absorbs carbon dioxide at low temperature (2–10°C). The low temperature limits the vaporization of ammonia in the absorber and entails precipitation of ammonium carbonate compounds, thereby allowing high loadings of CO$_2$. The process has thereby good perspectives. However, a scientific understanding and evaluation of the process is necessary. In this work, the performance of the carbon dioxide capture process using aqueous ammonia has been analyzed by process simulation. The Extended UNIQUAC thermodynamic model available for the CO$_2$–NH$_3$–H$_2$O system has been implemented in the commercial simulator Aspen Plus® by using a newly developed user model interface (Maribo-Mogensen et al., submitted for publication). It allows for making equilibrium calculations using the advanced thermodynamic model together with the features of the commercial simulator. The present work deals with the results from the process simulation study. Two process configurations have been tested and a thorough sensitivity analysis of the main process parameters has been performed in order to analyze their effects on the heat and electricity requirement. This work confirms the high potential of the process. The heat requirement is found to be in the same range as the values reported recently for advanced amine processes. Assuming that cold cooling water is available, the electricity consumption remains limited. Hence the Chilled Ammonia Process is a promising option for post combustion carbon dioxide capture.
Production Optimization for Two-Phase Flow In an Oil Reservoir

Petroleum reservoirs are subsurface formations of porous rocks with hydrocarbons trapped in the pores. Initially, the reservoir pressure may be sufficiently large to push the fluids to the production facilities. However, as the fluids are produced the pressure declines and production reduces over time. When the natural pressure becomes insufficient, the pressure must be maintained artificially by injection of water. Conventional technologies for recovery leaves more than 50% of the oil in the reservoir. Wells with adjustable downhole flow control devices coupled with modern control technology offer the potential to increase the oil recovery significantly. In optimal control of smart wells, downhole sensor equipment and remotely controlled valves are used in combination with large-scale subsurface flow models and gradient based optimization methods in a Nonlinear Model Predictive Control framework to increase the production and economic value of an oil reservoir. Wether the objective is to maximize recovery or some financial measure like Net Present Value, the increased production is achieved by manipulation of the well rates and bottom-hole pressures of the injection and production wells. The optimal water injection rates and production well bottom-hole pressures are computed by solution of a large-scale constrained optimal control problem. The objective is to maximize production by manipulating the well rates and bottom hole pressures of injection and production wells. Optimal control settings of injection and production wells are computed by solution of a large scale constrained optimal control problem. We describe a gradient based method to compute the optimal control strategy of the water flooding process. An explicit singly diagonally implicit Runge-Kutta
(ESDIRK) method with adaptive stepsize control is used for computationally efficient solution of the model. The gradients are computed by the adjoint method. The adjoint equations associated with the ESDIRK method are solved by integrating backwards in time. The necessary information for the adjoint computation is calculated and stored during the forward solution of the model. The backward adjoint computation then only requires the assembly of this information to compute the gradients.

Property Prediction for Emulsion based Chemical Product Design

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Center for Energy Resources Engineering, CERE – Center for Energy Resources Engineering
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Publication date: 2012
Event: Abstract from ANQUE ICCE 2012, Sevilla, Spain.
Main Research Area: Technical/natural sciences
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Publication: Research › Conference abstract for conference – Annual report year: 2012

Quantitative structure—property relationship for thermal decomposition temperature of ionic liquids
In this study, a wide literature survey has been conducted to gather an extensive set of thermal decomposition temperature (Td) data for ionic liquids (ILs). A data set consisting of Td data for 586 ILs was collated from 71 different...
literature sources. Using this data set, a reliable quantitative structure-property relationship has been developed. In order to consider the effects of the anion and cation on the Td of ILs, both anion-based and cation-based molecular descriptors were considered. Finally, a genetic function approximation method was used which selected 6 molecular descriptors for anions, and 6 molecular descriptors for cations to develop the model. The predictive capability of the 12-parameter model was evaluated using several validation techniques. Its applicability domain is discussed. The proposed model produces an acceptable average relative deviation of less than 5.2% taking into consideration all 586 experimental data values.

**General information**

State: Published

Organisations: Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering, University of KwaZulu-Natal, MINES ParisTech

Authors: Gharagheizi, F. (Ekstern), Sattari, M. (Ekstern), Ilani-Kashkouli, P. (Ekstern), Mohammadi, A. H. (Ekstern), Ramjugernath, D. (Ekstern), Richon, D. (Intern)

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Scopus rating (2007): SJR 1.347 SNIP 1.523
Real-Time Optimization for Economic Model Predictive Control

In this paper, we develop an efficient homogeneous and self-dual interior-point method for the linear programs arising in economic model predictive control. To exploit structure in the optimization problems, the algorithm employs a highly specialized Riccati iteration procedure. Simulations show that in comparison to conventional interior-point methods, our solver is a) significantly faster per. iteration and b) converges in a smaller and less fluctuating number of iterations.

General information
State: Published
Organisations: Department of Informatics and Mathematical Modeling, Scientific Computing, Computer Science and Engineering, Center for Energy Resources Engineering
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Number of pages: 8
Publication date: 2012

Selective oxidation of benzyl alcohol in dense CO2: Insight by phase behavior modeling
Catalytic reactions in pressurized CO2 are often strongly affected by the phase behavior. Knowledge on phase behavior is therefore desirable for optimizing the reaction conditions but often requires considerable experimental effort. Here, a previously established thermodynamic model for complex systems, based on the Cubic Plus Association (CPA) equation of state, is utilized in order to gain insight into the phase behavior during the palladium-catalyzed selective oxidation of benzyl alcohol to benzaldehyde. The catalytic reaction was studied in a tubular continuous reactor both under biphasic and single phase conditions at different flow rates, compositions and oxygen concentrations. In general, biphasic conditions resulted in the highest reaction rate which was also found when running the reaction in a batch reactor. On transition to a single phase a gradual deactivation of the catalyst was observed. Hence, the model predictions can be beneficially applied in order to find optimal reaction conditions. In the continuous reactor under biphasic conditions, the substrate was found to accumulate in the reactor due to segregation. The study indicates that a direct comparison between the catalytic performance observed in the continuous flow system and batch reactor under biphasic conditions requires knowledge on the influence of the segregation on flow conditions and mass transfer, which is often ignored in the literature.
Sequential Convex Programming for Power Set-point Optimization in a Wind Farm using Black-box Models, Simple Turbine Interactions, and Integer Variables

We consider the optimization of power set-points to a large number of wind turbines arranged within close vicinity of each other in a wind farm. The goal is to maximize the total electric power extracted from the wind, taking the wake effects that couple the individual turbines in the farm into account. For any mean wind speed, turbulence intensity, and direction we find the optimal static operating points for the wind farm. We propose an iterative optimization scheme to achieve this goal. When the complicated, nonlinear, dynamics of the aerodynamics in the turbines and of the fluid dynamics describing the turbulent wind fields' propagation through the farm are included in a highly detailed black-box model, numerical results for any given values of the parameter sets can easily be evaluated. However, analytic expressions for model representation in the optimization algorithms might be hard to derive and their properties are often not suitable for computationally efficient optimization either. To handle this, we propose a sequential convex optimization method, perturbing the model in each iteration, and demonstrate a typical convergence in fewer than 10 iterations. We derive a coupling matrix from the wind farm model, enabling us to use a very simple linear relationship for describing the turbine interactions. In addition, we allow individual turbines to be turned on or off introducing integer variables into the optimization problem. We solve this within the same framework of iterative convex approximation and compare with mixed-integer optimization tools. We demonstrate the method on a verified model and for various sizes and configurations of the wind farm. For all tested scenarios we observe a distribution of the power set-points which is at least as good as, and in many cases is far superior to, a more naive distribution scheme. We employ a fast convex quadratic programming solver to carry out the iterations in the range of microseconds for even large wind farms.

General information
State: Published
Organisations: Department of Informatics and Mathematical Modeling, Scientific Computing, Department of Electrical Engineering, Automation and Control, Center for Energy Resources Engineering, Vestas Technology R&D, Stanford University
Authors: Hovgaard, T. G. (Intern), Larsen, L. F. S. (Ekstern), Jørgensen, J. B. (Intern), Boyd, S. (Ekstern)
Number of pages: 8
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Optimization, Nonlinear Control, Wind Farms, Black-box Models, Integer Programming
Source: dtu
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Simulation, Control and Optimization of Single Cell Protein Production in a U-Loop Reactor

In 2011, the world population passed 7 billions inhabitants. While this number witnesses the success of humankind on earth, it also rises among other things questions about food supply. Declining live stock in the wild, rising price of energy combined with climatic change give a new economic potential for alternative sources of protein production. Single cell protein (SCP) is protein produced by growth of micro organisms. Among these micro organisms, Methylococcus Capsulatus is particular interesting as it can grow on either methane or methanol and contains 70% protein. The U-Loop reactor is particular useful for production of SCP by M. Capsulatus as it has good gas-liquid mass transfer capabilities and also the capability to remove the significant amount of heat developed by the reaction. In this paper we describe an implementation of a model to simulate SCP production in the U-Loop reactor. We report simulation results. In addition we design and compare dierent regulatory control systems for regulation of SCP production in the U-Loop reactor. The purpose of the regulatory control systems is to keep the process at a steady state and to reject disturbances. We design and implement such control systems based upon PID and MPC technology. In particular, we design these control systems such that they can be used as the regulatory layer in a process control hierarchy and enable resilient transition from one operating point to another. The optimal operating points are determined by the real-time optimization (RTO) part of the control system.
Single Shooting and ESDIRK Methods for adjoint-based optimization of an oil reservoir

Conventional recovery techniques enable recovery of 10-50% of the oil in an oil field. Advances in smart well technology and enhanced oil recovery techniques enable significant larger recovery. To realize this potential, feedback model-based optimal control technologies are needed to manipulate the injections and oil production such that flow is uniform in a given geological structure. Even in the case of conventional water flooding, feedback-based optimal control technologies may enable higher oil recovery than with conventional operational strategies. The optimal control problems that must be solved are large-scale problems and require specialized numerical algorithms. In this paper, we combine a single shooting optimization algorithm based on sequential quadratic programming (SQP) with explicit singly diagonally implicit Runge-Kutta (ESDIRK) integration methods and a continuous adjoint method for sensitivity computation. We demonstrate the procedure on a water flooding example with conventional injectors and producers.
Solids Modelling and Capture Simulation of Piperazine in Potassium Solvents

Piperazine is an amine which is used both as an activator or promoter, but also as active component in CO2 capture solvents. High concentrations are being formulated to draw benefit of the PZ properties. This results in a risk of precipitation of PZ and other solid phases during capture. It could be a benefit to the capture process, but it could also result in unforeseen situations of potential hazardous operation, clogging, equipment failure etc. Security of the PZ process needs to be in focus. Flow assurance requires additional attention, especially due to the precipitation phenomenon. This entails all parts of the streams, but also during formulation and transport of the solvent. In this work the extended UNIQUAC thermodynamic model is presented with the addition of piperazine (PZ or PIPH2) in combination with the potassium ion of mixtures with CO2 in equilibration with KOH-KHCO3-K2CO3. Phase boundaries are laid out which shows the concentration regions of solid formation. A special focus will be given to the boundary where precipitations occur. The model is a generic. It builds on consistent parameters of the extended UNIQUAC model previously published. It allows for accurate vapor liquid equilibrium (VLE) calculation, heat capacity determination, and similar thermodynamic properties. It especially allows for determination of solid liquid equilibria (SLE) and heat of absorption/heat of desorption which are core variables in the determination of energy requirements for CO2 capture. In this work the typical phase behavior will be shown for the PZ solvent with potassium (K2CO3/KHCO3) for CO2 capture. Conclusions are given on a solvent compositions resulting in low heat requirements using the predictive nature of the extended UNIQUAC model. Concentration of a PZ/K2CO3 solvent is suggested with a heat of absorption/desorption of 40kJ/mol.
Solubilities of ferrocene and acetylferrocene in supercritical carbon dioxide

In this work, the solubilities of ferrocene and acetylferrocene in supercritical carbon dioxide (scCO2) were measured using an analytical method in a quasi-flow apparatus. High-performance liquid chromatography was applied through an online sampling procedure to determine the concentration of ferrocene and acetylferrocene in the scCO2 phase. The experiments were performed within a temperature range of 308–348K and at pressures ranging from 7.7 to 24.4MPa. Acetylferrocene is the product of the Friedel–Crafts acylation reaction of ferrocene and has many applications in the material and pharmaceutical industries. The molar solubilities at the applied conditions range from 8.9 to 31.2×10−4 for ferrocene and 2.5 to 79.2×10−4 for acetylferrocene. The existence of a cross-over area for acetylferrocene was detected at a pressure of around 15MPa and for ferrocene at a pressure of around 10MPa. The comparison between the experimental solubility data shows that ferrocene is more soluble in scCO2 at lower pressures, while at higher pressures acetylferrocene is more soluble in scCO2. The reason for this behavior is a trade-off between the lower polarity of ferrocene (more dominant at lower pressures) and the higher volatility of acetylferrocene (more dominant at higher pressures). Results obtained in this work show that the solubility of the reaction product acetylferrocene in scCO2 is sufficiently high to use scCO2 extraction at high pressures to separate it from its reactant ferrocene in Friedel–Crafts acylation processes.
In this paper, we describe a novel numerical algorithm for solution of constrained optimal control problems of the Bolza type for stiff and/or unstable systems. The numerical algorithm combines explicit singly diagonally implicit Runge-Kutta (ESDIRK) integration methods with a multiple shooting algorithm. As we consider stiff systems, implicit solvers with sensitivity computation capabilities for initial value problems must be used in the multiple shooting algorithm. Traditionally, multi-step methods based on the BDF algorithm have been used for such problems. The main novel contribution of this paper is the use of ESDIRK integration methods for solution of the initial value problems and the corresponding sensitivity equations arising in the multiple shooting algorithm. Compared to BDF-methods, ESDIRK-methods are advantageous in multiple shooting algorithms in which restarts and frequent discontinuities on each shooting interval are present. The ESDIRK methods are implemented using an inexact Newton method that reuses the factorization of the iteration matrix for the integration as well as the sensitivity computation. Numerical experiments are provided to demonstrate the algorithm.
State Estimation for the Automotive SCR Process

Selective catalytic reduction (SCR) of NOx is a widely applied diesel engine exhaust gas aftertreatment technology. For advanced SCR process control, like model predictive control, full state information of the process is required. The ammonia coverage ratio inside the catalyst is difficult to measure. Therefore we design an ordinary Kalman filter as well as an extended Kalman filter to estimate the ammonia coverage. The filters are built over a first principle model with four states. Among the four states, NO, NO2 and NH3 concentration are measured by the sensors, while the ammonia coverage ratio is left to be unknown. The performance of the filters is shown by simulation with the World Harmonized transient cycle. In particular, during transient operations the extended Kalman filter performs significantly better than the ordinary Kalman filter. Since such operation regimes are always present for SCR in engine applications, we recommend estimating the ammonia coverage using the extended Kalman filter.

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, Scientific Computing, Department of Informatics and Mathematical Modeling, Center for Energy Resources Engineering, Technical University of Denmark
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State Estimation in the Automotive SCR DeNOx Process

Selective catalytic reduction (SCR) of nitrogen oxides (NOx) is a widely applied diesel engine exhaust gas after-treatment technology. For effective NOx removal in a transient operating automotive application, controlled dosing of urea can be used to meet the increasingly restrictive legislations on exhaust gas emissions. For advanced control, e.g. Model Predictive Control (MPC), of the SCR process, accurate state estimates are needed. We investigate the performance of the ordinary and the extended Kalman filters based on a simple first principle system model. The performance is tested through a series of simulation studies reflecting realistic challenges such as under-modelling and few gas composition sensors.

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State Estimation in the Automotive SCR DeNOx Process

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Organisations: Center for Energy Resources Engineering, Department of Informatics and Mathematical Modeling, Scientific Computing, Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, CHEC Research Centre, Haldor Topsoe AS
Authors: Zhou, G. (Intern), Jørgensen, J. B. (Intern), Duwig, C. (Ekstern), Huusom, J. K. (Intern)
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Static and dynamic effective stress coefficient of chalk
Deformation of a hydrocarbon reservoir can ideally be used to estimate the effective stress acting on it. The effective stress in the subsurface is the difference between the stress due to the weight of the sediment and a fraction (effective stress coefficient) of the pore pressure. The effective stress coefficient is thus relevant for studying reservoir deformation and for evaluating 4D seismic for the correct pore pressure prediction. The static effective stress coefficient $n$ is estimated from mechanical tests and is highly relevant for effective stress prediction because it is directly related to mechanical strain in the elastic stress regime. The corresponding dynamic effective stress coefficient $\alpha$ is easy to estimate from density and velocity of acoustic (elastic) waves. We studied $n$ and $\alpha$ of chalk from the reservoir zone of the Valhall field, North Sea, and found that $n$ and $\alpha$ vary with differential stress (overburden stress-pore pressure). For Valhall reservoir chalk with 40% porosity, $\alpha$ ranges between 0.98 and 0.85 and decreases by 10% if the differential stress is increased by 25 MPa. In contrast, for chalk with 15% porosity from the same reservoir, $\alpha$ ranges between 0.85 and 0.70 and decreases by 5% due to a similar increase in differential stress. Our data indicate that $\alpha$ measured from sonic velocity data falls in the same range as for $n$, and that $n$ is always below unity. Stress-dependent behavior of $n$ is similar (decrease with increasing differential stress) to that of $\alpha$ during elastic deformation caused by pore pressure buildup, for example, during waterflooding. By contrast, during the increase in differential stress, as in the case of pore pressure depletion due to production, $n$ increases with stress while $\alpha$ decreases.

General information
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Organisations: Department of Civil Engineering, Section for Geotechnics and Geology, Center for Energy Resources Engineering, Danish Geotechnical Institute
Authors: Alam, M. M. (Intern), Fabricius, I. L. (Intern), Christensen, H. F. (Ekstern)
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Main Research Area: Technical/natural sciences
Stochastic Model Predictive Control with Applications in Smart Energy Systems

In response to growing concerns related to environmental issues, limited resources and security of supply, the energy industry is changing. One of the most significant developments has been the penetration of renewable energy sources. In Denmark, the share of wind power generation is expected to cover more than 50% of the total consumption by 2050. Energy systems based on significant amounts of renewable energy sources are subject to uncertainties. To accommodate the need for model predictive control (MPC) of such systems, the effect of the stochastic effects on the constraints must be accounted for. In conventional MPC, the stochastic effects on the constraints is handled by constraint back-off and the MPC problem can still be solved by solution of either a linear program or a quadratic program. Treating the constraints as probabilistic constraints provides a more systematic approach to handle the stochastic effects on constraints. In this formulation, the MPC may be represented by a chance constrained mathematical program. The chance constraints allow a direct tradeoff between a certain (low) frequency of violating the constraints and a performance function (e.g. an economic loss function). This is convenient for energy systems, since some constraints are very important to satisfy with a high probability, whereas violation of others are less prone to have a large economic penalty. In MPC applications the control action is obtained by solving an optimization problem at each sampling instant. To make the controller applicable in real-time efficient and reliable algorithms are required. If the uncertainty is assumed to be Gaussian, the optimization problems associated with chance constrained (linear) MPC can be expressed as second order cone programming (SOCP) problems. In this paper, we show that tailored interior point algorithms are well suited to handle this type of problems. Namely, by utilizing structure-exploiting methods, we implement a special-purpose solver for control of smart energy systems. The solver is compared against general-purpose implementations. As a case study, we consider a system consisting of fuel-fired thermal power plants, wind farms and electric vehicles.

Systematic identification of crystallization kinetics within a generic modelling framework

A systematic development of constitutive models within a generic modelling framework has been developed for use in design, analysis and simulation of crystallization operations. The framework contains a tool for model identification connected with a generic crystallizer modelling tool-box, a tool for data handling and translation as well as model application features. Through this framework it is possible, for a wide range of crystallization processes, to generate the necessary problem-system specific models; to identify the parameters for constitutive models; and to handle or translate raw crystallization data. Application of the systematic framework is highlighted through a sucrose crystallization case study, for which the parameters for nucleation and crystal growth are first estimated from the available measured data and are then applied to study the crystallization operation.
The Conversion of Cardiovascular Conference Abstracts to Publications

**Background**—The transition of scientific knowledge from discovery into practice is less than ideal. A key step in this translation occurs when presentations from major meetings are published in peer-reviewed literature, yet the completeness and speed of this process are not known. We performed a systematic and automated evaluation of rates, timing, and correlates of publication from scientific abstracts presented at 3 major cardiovascular conferences.

**Methods and Results**—Using an automated computer algorithm, we searched the ISI Web of Science to identify peer-reviewed publications of abstracts presented at the American Heart Association (AHA), American College of Cardiology (ACC), and European Society of Cardiology (ESC) scientific sessions from 2006 to 2008. We compared abstract publication rates and journal impact factor between the 3 meetings using multivariable logistic regression modeling. From 2006 to 2008, 11,365, 5005, and 10,838 abstracts were presented at the AHA, ACC, and ESC meetings, respectively. Overall, 30.6% of presented abstracts were published within 2 years of the conference; ranging from 34.5% for AHA to 29.5% for ACC to 27.0% for ESC (P < 0.0001). Five years after conference presentation in 2005, these rates had risen slightly to 49.7% for AHA, 42.6% for ACC, and 37.6% for ESC (P < 0.0001). After adjustment for abstract characteristics and contributing countries, abstracts presented at the AHA meeting remained more likely for publication relative to the ESC (adjusted odds ratio, 1.24; 95% confidence interval, 1.16–1.34) and the ACC (adjusted odds ratio, 1.20; 95% confidence interval, 1.11–1.29). Median impact factors for subsequent publications varied from 4.8 (interquartile range, 3.8–10.1) for AHA to 4.0 (interquartile range, 3.1–7.5) for ACC and 3.9 (quartile 1–3, 2.5–5.8) for ESC (P for difference between groups 0.01). Clinical science and population science were less likely to be published compared with basic science.

**Conclusions**—One third of abstracts were translated into publications by 2 years after presentation and less than one half by 5 years after presentation. Our findings suggest that efforts to understand the barriers to publication and to facilitate the rapid dissemination of new knowledge are needed to speed up the transition of scientific discovery into clinical practice.
The effect of pressure on the phase behavior of surfactant systems: An experimental study

Enhanced oil recovery is employed in many mature oil reservoirs to maintain or increase the reservoir recovery factor. In this context, surfactant flooding has recently gained interest again. Surfactant flooding is the injection of surfactants (and co-surfactants) into the reservoir, in order to create microemulsions at the interface between crude oil and water, thus obtaining very low interfacial tension, which consequently helps mobilize the trapped oil. In this work a surfactant system, which has been thoroughly described at atmospheric pressure, is examined at elevated pressure. The effect of temperature is also explored. It was found that the phase behavior in the system water/sodium dodecyl sulfate (SDS)/1-butanol/heptane/sodium chloride was significantly changed by an increase in pressure. When an increase in pressure is combined with an increased temperature the phase behavior of the system is influenced to an even greater extent. It was concluded that at certain compositions of the surfactant system (near to the phase boundary found at atmospheric pressure) the increase in pressure changed the phase behavior (for example causing the system to move from two phases to three or vice versa). The sensitivity of the surfactant system depends very much on the overall composition as well as the magnitude of the pressure and temperature change.

General information
State: Published
Organisations: Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering, Department of Chemistry
Authors: Sandersen, S. B. (Intern), Stenby, E. H. (Intern), von Solms, N. (Intern)
Pages: 159-166
Publication date: 2012
Main Research Area: Technical/natural sciences
The Influence of Biot's Coefficient on the Estimation of Effective Stress on Deep Sea Sediments

In this paper we address the changes in physical properties of the Eocene and Paleocene shale from the Atlantic Basin, as a function of burial diagenesis. We also showed the influence of using correct Biot's coefficient (β) on the estimation of vertical effective stress. We correlated our porosity and P-wave velocity data with the calculated effective stresses to show how different calculated vertical effective stress influences shale compaction trends. This may provide a basis to understand how physical properties vary with effective stress and shale mineralogy. Our results may be relevant for drilling, basin analysis modeling, seismic interpretation and hydrocarbon exploration.

General information
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Organisations: Department of Civil Engineering, Section for Geotechnics and Geology, Center for Energy Resources Engineering
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Main Research Area: Technical/natural sciences

Thermally Induced Permeability Reduction due to Particle Migration in Sandstones: The Effect of Temperature on Kaolinite Mobilisation and Aggregation

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering
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Thermodynamically Based Solvent Design for Enzymatic Saccharide Acylation with Hydroxycinnamic Acids in Non-conventional Media

Enzyme-catalyzed synthesis has been widely studied with lipases (EC 3.1.1.3), but feruloyl esterases (FAEs; EC 3.1.1.73) may provide advantages such as higher substrate affinity and regioselectivity in the synthesis of hydroxycinnamate saccharide esters. These compounds are interesting because of their amphiphilicity and antioxidative potential. Synthetic reactions using mono- or disaccharides as one of the substrates may moreover direct new routes for biomass upgrading in the biorefinery. The paper reviews the available data for enzymatic hydroxycinnamate ester synthesis in organic solvent systems as well as other enzymatic hydroxycinnamate acylations in ionic liquid systems. The choice of solvent system is highly decisive for enzyme stability, selectivity, and reaction yields in these synthesis reactions. To increase the understanding of the reaction environment and to facilitate solvent screening as a crucial part of the reaction design, the review explores the use of activity coefficient models for describing these systems and – more importantly – the use of group contribution model UNIFAC and quantum chemistry based COSMO-RS for thermodynamic predictions and preliminary solvent screening. Surfactant-free microemulsions of a hydrocarbon, a polar alcohol, and water are interesting solvent systems because they accommodate different substrate and product solubilities and maintain enzyme stability. Ionic liquids may provide advantages as solvents in terms of increased substrate and product solubility, higher reactivity and selectivity, as well as tunable physicochemical properties, but their design should be carefully considered in relation to enzyme stability. The treatise shows that thermodynamic modeling tools for solvent design provide a new toolbox to design enzyme-catalyzed synthetic reactions from biomass sources.
Thermodynamic modeling of phase equilibria of semi-clathrate hydrates of CO$_2$, CH$_4$, or N$_2$+tetra-n-butylammonium bromide aqueous solution

Prediction of phase equilibria of semi-clathrate hydrates has been very rarely investigated in the literature. In this work, a thermodynamic model is proposed for representation/prediction of phase equilibria of semi-clathrate hydrates of the CO$_2$, CH$_4$, or N$_2$+tetra-n-butylammonium bromide (TBAB) aqueous solution. For modeling the hydrate phase, the van der Waals–Platteeuw (vdW–P) solid solution theory is used, revised with two modifications for evaluations of Langmuir constants and vapor pressure of water in the empty hydrate lattice, in which these values are supposed to be a function of TBAB concentration in aqueous solution. The Peng–Robinson (PR-EoS) equation of state along with re-tuned parameters of Mathias–Copeman alpha function is applied for calculation of the fugacity of gaseous hydrate former. For determination of the activity coefficient of the non-electrolyte species in the aqueous phase, the Non-Random Two-Liquid (NRTL) activity model is used. To calculate the mean activity coefficients of the electrolyte portion, a correlation on the basis of existing osmotic coefficient and activity coefficient values is employed. It is shown that the presented model results are in acceptable agreement with the experimental semi-clathrate hydrate dissociation data investigated in this work.

General information
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Organisations: Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering, MINES ParisTech
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Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
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Web of Science (2014): Indexed yes
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Highlights.
- A thermodynamic model is proposed for investigation of semi-clathrate hydrates.
- The studied systems include CO2, CH4, or N2+TBAB aqueous solution.
- The vdW–P theory along with two modifications are used for hydrate phase.
- The PR EoS and NRTL activity model are applied for modeling the fluid phases.
- Promotion/inhibition effects of TBAB can be well determined using the model.

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Thirty Years with EoS/GE Models - What Have We Learned?
Thirty years of research and the use of EoS/GE mixing rules in cubic equations of state are reviewed. The most popular approaches are presented both from the derivation and application points of view and they are compared to each other. It is shown that all methods have significant capabilities but also limitations which are discussed. A useful approach is presented for analyzing the models by looking at the activity coefficient expression derived from the equations of state using various mixing rules. The size-asymmetric systems are investigated in detail, and an explanation is provided on how EoS/GE mixing rules should be developed so that such asymmetric mixtures are adequately represented. © 2012 American Chemical Society.

General information
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Organisations: Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering, Technical University of Denmark
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Web of Science (2014): Indexed yes
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Scopus rating (2013): SJR 0.982 SNIP 1.243 CiteScore 2.6
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BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.066 SNIP 1.338 CiteScore 2.56
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ISI indexed (2011): ISI indexed yes
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Scopus rating (2010): SJR 1.047 SNIP 1.165
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Scopus rating (2009): SJR 1.002 SNIP 1.164
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 1.142 SNIP 1.267
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Web of Science (2007): Indexed yes
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Web of Science (2006): Indexed yes
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Web of Science (2004): Indexed yes
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Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 1.372 SNIP 1.41
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Transport properties of natural gas through polyethylene nanocomposites at high temperature and pressure

High density polyethylene (HDPE)/clay nanocomposites containing nanoclay concentrations of 1, 2.5, and 5 wt% were prepared by a melt blending process. The effects of various types of nanoclays and their concentrations on permeability, solubility, and diffusivity of natural gas in the nanocomposites were investigated. The results were compared with HDPE typically used in the production of liners for the petroleum industry. Four different nanoclays—Cloisite 10A, 15A, 30B and Nanomer 1.44P—were studied in the presence of CH₄ and a CO₂/CH₄ mixture in the temperature range 30-70 degrees C and pressure range 50-100 bar. The permeability and diffusivity of the gases were considerably reduced by the incorporation of nanoclay into the polymer matrix. Addition of 5 wt% loading of Nanomer 1.44P reduced the permeability by 46% and the diffusion coefficient by 43%. Increasing the pressure from 50 to 100 bar at constant temperature had little influence on the permeability, whereas increasing the temperature from 30 to 70 degrees C significantly increased the permeability of the gas. Additionally, the effect of crystallinity on permeability, solubility, and diffusivity was investigated. Thus, the permeability of the CO₂/CH₄ mixture in Nanomer 1.44P nanocomposite was reduced by 47% and diffusion coefficient by 35% at 5 wt% loading, 50 degrees C, and 100 bar, compared with pure HDPE.
Tuning of Controller for Type 1 Diabetes Treatment with Stochastic Differential Equations

People with type 1 diabetes need several insulin injections every day to keep their blood glucose level in the normal range and thereby avoiding the acute and long term complications of diabetes. One of the recent treatments consists of a pump injecting insulin into the subcutaneous layer combined with a continuous glucose monitor (CGM) frequently observing the glucose level. Automatic control of the insulin pump based on CGM observations would ease the burden of constant diabetes treatment and management. We have developed a controller designed to keep the blood glucose level in the normal range by adjusting the size of insulin infusions from the pump based on model predictive control (MPC). A clinical pilot study to test the performance of the MPC controller overnight was performed. The conclusion was that the controller relied too much on the local trend of the blood glucose level which is a problem due to the noise corrupted observations from the CGM. In this paper we present a method to estimate the optimal Kalman gain in the controller based on stochastic differential equation modeling. With this model type we could estimate the process noise and observation noise separately based on data from the rst clinical pilot study. In doing so we obtained a more robust control algorithm which is less sensitive to fluctuations in the CGM observations and rely more on the global physiological trend of the blood glucose level. Finally, we present the promising results from the second pilot study testing the improved controller.
Tuning SISO offset-free Model Predictive Control based on ARX models

In this paper, we present a tuning methodology for a simple offset-free SISO Model Predictive Controller (MPC) based on autoregressive models with exogenous inputs (ARX models). ARX models simplify system identification as they can be identified from data using convex optimization. Furthermore, the proposed controller is simple to tune as it has only one free tuning parameter. These two features are advantageous in predictive process control as they simplify industrial commissioning of MPC. Disturbance rejection and offset-free control is important in industrial process control. To achieve offset-free control in face of unknown disturbances or model-plant mismatch, integrators must be introduced in either the estimator or the regulator. Traditionally, offset-free control is achieved using Brownian disturbance models in the estimator. In this paper we achieve offset-free control by extending the noise model with a filter containing an integrator. This filter is a first order ARMA model. By simulation and analysis, we argue that it is independent of the parameterization of the underlying linear plant; while the tuning of traditional disturbance models is system dependent. Using this insight, we present MPC for SISO systems based on ARX models combined with the first order filter. We derive expressions for the closed-loop variance of the unconstrained MPC based on a state space representation in innovation form and use these expressions to develop a tuning procedure for the regulator. We establish formal equivalence between GPC and state space based off-set free MPC. By simulation we demonstrate this procedure for a third order system. The offset-free ARX MPC demonstrates satisfactory set point tracking and rejection of an unmeasured step disturbance for a simulated furnace with a long time delay.

General information
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Vapor–Liquid–Liquid Equilibrium Measurements and Modeling of the Methanethiol + Methane + Water Ternary System at 304, 334, and 364 K

New vapor–liquid–liquid equilibrium (VLLE) data for methanethiol (CH$_3$SH) + methane (CH$_4$) + water (H$_2$O) have been obtained at three temperatures (304, 334, and 364 K) and pressures up to 9 MPa. A “static-analytical” method was used to perform all of the measurements. The objective was to provide experimental VLLE data for CH$_3$SH with other natural gas contents at its crude form for which limited or no data are available in the open literature. Such kinds of data are required for the industrial modeling of sulfur emissions. It is observed from the experimental data that the solubility of CH$_4$ in the aqueous and organic phases increases with an increase of the total system pressure and decreases with an increase of the temperature. However, the solubility of CH$_3$SH in the aqueous and organic phases decreases slightly with an increase of the total system pressure and increases significantly with an increase of the temperature. The new VLLE data of this ternary system were compared with predictions of the cubic-plus-association equation of state. The model tends to underpredict the concentration of CH$_3$SH in all phases, particularly the vapor phase.

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Organisations: Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Ressources Engineering, MINES ParisTech
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Vp-Vs relationship and amplitude variation with offset modelling of glauconitic greensand

The relationship between Vp and Vs may be used to predict Vs where only Vp is known. Vp/Vs is also used to identify pore fluids from seismic data and amplitude variation with offset analysis. Theoretical, physical, as well as statistical empirical Vp-Vs relationships have been proposed for reservoir characterization when shearwave data are not available. In published work, the focus is primarily on the Vp-Vs relationship of quartzitic sandstone. In order to broaden the picture we present Vp-Vs relationships of greensand composed of quartz and glauconite by using data from the Paleocene greensand Nini oil field in the North Sea. A Vp-Vs relationship derived from modelling is compared with empirical Vp-Vs regressions from laboratory data as well as from log data. The accuracy of Vs prediction is quantified in terms of rootmean-square error. We find that the Vp-Vs relationship derived from modelling works well for greensand shear-wave velocity prediction. We model the seismic response of glauconitic greensand by using laboratory data from the Nini field. Our studies here reveal that brine-saturated glauconitic greensand can have a similar seismic response to that from oil-saturated quartzitic sandstone and that oil-saturated strongly cemented greensand can have a similar amplitude variation with offset response to that from brine-saturated weakly cemented greensand.

General information
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BFI (2015): BFI-level 1
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Scopus rating (2012): SJR 1.147 SNIP 1.312 CiteScore 1.39
ISI indexed (2012): ISI indexed yes
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BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.823 SNIP 1.347 CiteScore 1.92
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Wettability Improvement with Enzymes: Application to Enhanced Oil Recovery under Conditions of the North Sea Reservoirs

Enzymes are well-known biological agents and have been applied previously in the petroleum industry. However, only recently they have been introduced into the field of enhanced oil recovery (EOR). Although initially reported results of the application of enzymes for EOR are quite positive and promising (Nasiri et al., 2009), working mechanisms are poorly known and understood. The main goal of the present work is to establish possible mechanisms in which enzymes may enhance oil recovery.

Improvement of the brine wettability of the rock and decrease of oil adhesion to it by addition of an enzyme is one of the possible mechanisms of enzymatic action. This mechanism has been investigated experimentally, by measurements of the contact angles between oil drops and enzyme solutions in brine on the mineral surfaces.

Fifteen enzyme samples belonging to different enzyme classes, such as esterases/lipases, carbohydrases, proteases and oxidoreductases, provided by Novozymes, have been investigated. Two commercial mixtures containing enzymes: Apollo-GreenZyme™ and EOR-ZYMAX™ have also been applied. The North Sea dead oil and the synthetic sea water were used as test fluids. Internal surface of a carbonate rock has been mimicked using calcite crystals.

Overall, the group of esterases/lipases has demonstrated the best performance in terms of wettability alteration. Particularly, a non-specific esterase product has been found to turn the mineral surfaces into non-adhesive state at concentrations of 0.1-0.5% wt. Proteases appear to be relatively ambiguous, while carbohydrases and oxidoreductases have the lowest potential for EOR in the light of the present experiments. Suggested mechanisms for wettability improvement for esterases/lipases are adsorption of enzymes onto the mineral and/or formation of additional interfacially active oil compounds. Application of the commercial product Apollo-GreenZyme™ has also resulted in positive wettability changes, but according to the observations the working mechanisms are different. In an attempt to assess validity of the proposed mechanisms, the reference experiments have been conducted with concentrated enzymes, enzyme product stabilizers, surfactant and protein.

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Source-ID: 316451
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2011

Adaptive Disturbance Estimation for Offset-Free SISO Model Predictive Control

Offset free tracking in Model Predictive Control requires estimation of unmeasured disturbances or the inclusion of an integrator. An algorithm for estimation of an unknown disturbance based on adaptive estimation with time varying forgetting is introduced and benchmarked against the classical disturbance modelling approach, where the system description is augmented by a disturbance state. The time varying forgetting renders the new approach less sensitive to the nature of the disturbance. By simulation we demonstrate that this algorithm is advantageous in case of infrequent step disturbances of any magnitude.

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Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, Mathematical Statistics, Department of Informatics and Mathematical Modeling, Scientific Computing, Center for Energy Resources Engineering
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Advanced Waterflooding in Chalk Reservoirs: Crude Oil/Brine Interaction Study

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Organisations: Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering, Department of Chemistry
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Advanced waterflooding in chalk reservoirs: Understanding of underlying mechanisms

Over the last decade, a number of studies have shown SO$_4^{2-}$, Ca$^{2+}$ and Mg$^{2+}$ to be potential determining ions, which may be added to the injected brine for improving oil recovery during waterflooding in chalk reservoirs. However the understanding of the mechanism leading to an increase in oil recovery is still not clear. In this work the crude oil/seawater ions interaction at different temperatures, pressures and sulfate ion concentrations is investigated. Our results show that sulfate ions may help decrease the crude oil viscosity when brine is contacted with oil under high temperature and pressure. We have also observed formation of a microemulsion phase between brine and oil with the increase in sulfate ion concentration at high temperature and pressure. In addition, sulfate ions can reduce interfacial tension (IFT) between oil and water. We propose that the decrease in viscosity and formation of a microemulsion phase could be the possible reasons for the observed increase in oil recovery with sulfate ions at high temperature in chalk reservoirs besides the mechanism of the rock wettability alteration, which has been reported in most previous studies.
A Frequency Matching Method for Generation of a Priori Sample Models from Training Images
This paper presents a Frequency Matching Method (FMM) for generation of a priori sample models based on training images and illustrates its use by an example. In geostatistics, training images are used to represent a priori knowledge or expectations of models, and the FMM can be used to generate new images that share the same multi-point statistics as a given training image. The FMM proceeds by iteratively updating voxel values of an image until the frequency of patterns in the image matches the frequency of patterns in the training image; making the resulting image statistically indistinguishable from the training image.

A Mathematical Model for Non-monotonic Deposition Profiles in Deep Bed Filtration Systems
A mathematical model for suspension/colloid flow in porous media and non-monotonic deposition is proposed. It accounts for the migration of particles associated with the pore walls via the second energy minimum (surface associated phase). The surface associated phase migration is characterized by advection and diffusion/dispersion. The proposed model is able to produce a nonmonotonic deposition profile. A set of methods for estimating the modeling parameters is provided in the case of minimal particle release. The estimation can be easily performed with available experimental information. The numerical modeling results highly agree with the experimental observations, which proves the ability of the model to catch a non-monotonic deposition profile in practice. An additional equation describing a mobile population behaving differently
from the injected population seems to be a sufficient condition for producing non-monotonic deposition profiles. The described physics by the additional equation may be different in different experimental settings.
Amino acid salt solutions as solvents in CO2 capture from flue gas: CO2 loading capacity and precipitation.

New solvents based on the salts of amino acids have emerged as an alternative to the alkanolamine solutions, for the chemical absorption of CO2 from flue gas. But only few studies on amino acids as CO2 capturing agents have been performed so far. One of the interesting features of amino acid salt solutions is their ability to form solid precipitates upon the absorption of CO2. The occurrence of crystallization offers the possibility of increasing the CO2 loading capacity of the solvent. However, precipitation can also have negative effect on the CO2 capture process. The chemical nature of the solid formed is a decisive factor in determining the effect of precipitation on the process. For the purpose of studying the CO2 loading capacity of amino acid salt solutions, we developed an experimental set-up based on a dynamic analytical mode, with analysis of the effluent gas. Using this set-up, the CO2 loading capacity of aqueous solutions of the potassium salts of selected amino-acids (glycine, taurine, lysine proline, and glutamic acid) were examined, and the relation between the initial amino acid salt concentration and precipitation ability of each solution were determined. Experiments were performed at a partial pressure of CO2 close to 10 kPa, and a total pressure around 100 kPa, and a temperature close to 298 K. The obtained precipitates were analyzed using X-ray diffraction and infra-red spectroscopy. It was verified that the precipitate consisted of the amino acid itself in the case of glycine, taurine, and lysine, while in the case of proline, and glutamic acid, the precipitate was found to be bicarbonate. These results give an important contribution to further understanding the potential of amino acid salt solutions in CO2 capture from flue gas.

Aqueous Solubility of Piperazine and 2-Amino-2-methyl-1-propanol plus Their Mixtures Using an Improved Freezing-Point Depression Method

In this work the solid–liquid equilibrium (SLE) and freezing-point depression (FPD) in the electrolytic binary aqueous systems piperazine (PZ, CAS No. 110-85-0) and aqueous 2-amino-2-methyl-1-propanol (AMP, CAS No. 124-68-5) were measured. The FPD and solubility were also determined in the ternary AMP–PZ–H2O system. A method was developed by which solubility can be determined at higher temperatures using the FPD setup. A total of 86 data points are listed in the full concentration range from (−35 to 90) °C. The solid phases piperazine hexahydrate (PZ·6H2O), piperazine hemihydrate (PZ·1/2H2O), and anhydrous PZ precipitated during the experiments. The data can be used in the formulation, prevention, or intentional formation of slurries in piperazine solvents for promoting CO2 capture using absorption and desorption.

General information
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Authors: Lerche, B. M. (Intern), Thomsen, K. (Intern), Stenby, E. H. (Intern)
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Aqueous Solubility of Piperazine and 2-Amino-2-methyl-1-propanol plus Their Mixtures Using an Improved Freezing-Point Depression Method

In this work the solid–liquid equilibrium (SLE) and freezing-point depression (FPD) in the electrolytic binary aqueous systems piperazine (PZ, CAS No. 110-85-0) and aqueous 2-amino-2-methyl-1-propanol (AMP, CAS No. 124-68-5) were measured. The FPD and solubility were also determined in the ternary AMP–PZ–H2O system. A method was developed by which solubility can be determined at higher temperatures using the FPD setup. A total of 86 data points are listed in the full concentration range from (−35 to 90) °C. The solid phases piperazine hexahydrate (PZ·6H2O), piperazine hemihydrate (PZ·1/2H2O), and anhydrous PZ precipitated during the experiments. The data can be used in the formulation, prevention, or intentional formation of slurries in piperazine solvents for promoting CO2 capture using absorption and desorption.

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Web of Science (2016): Indexed yes
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Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.021 SNIP 1.208 CiteScore 2.22
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.135 SNIP 1.199 CiteScore 2.17
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.141 SNIP 1.103 CiteScore 2.01
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
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ISI indexed (2011): ISI indexed yes
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Scopus rating (2010): SJR 1.054 SNIP 1.299
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Bibliographical note
Special Issue: Kenneth N. Marsh Festschrift
Biot critical frequency applied as common friction factor for pore collapse and failure of chalk with different pore fluids and temperatures

A fluid effect toward higher strengths for oil-saturated chalk compared with water-saturated chalk has previously been identified and labeled the "water-weakening phenomenon," but has not been further characterized physically. The hypothesis of this paper is that the Biot critical frequency with a strain or stress-rate dependence can be used to explain this behavior on the pore scale and can be extrapolated to the macroscale failure and pore-collapse properties. A large set of previously published laboratory test results on chalk with different pore fluids was collected, and as a supplement we present a new test series on Stevns chalk with unconfined compression and Brazilian strength results. Copyright © 2011 Society of Petroleum Engineers.
Building a multilevel modeling network for lipid processing systems

The aim of this work is to present the development of a computer aided multilevel modeling network for the systematic design and analysis of processes employing lipid technologies. This is achieved by decomposing the problem into four levels of modeling: i) pure component property modeling and a lipid-database of collected experimental data from industry and generated data from validated predictive property models, as well as modeling tools for fast adoption-analysis of property prediction models; ii) modeling of phase behavior of relevant lipid mixtures using the UNIFAC-CI model, development of a master parameter table and calculations of the activity coefficients (VLE) related to a multicomponent system; iii) development of a model library consisting of new and adopted process models of unit operations involved in lipid processing technologies, validation of the developed models using operating data collected from existing process plants, and application of validated models in design and analysis of unit operations; iv) the information and models developed are used as building blocks in the development of methods and tools for computer-aided synthesis and design of process flowsheets (CAFD). The applicability of this methodology is highlighted in each level of modeling through the analysis of a lipid process that has significant relevance in the edible oil and biodiesel industries since it determines the quality of the final oil product, the physical refining process of oils and fats.

General information

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Organisations: Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, CERE – Center for Energy Ressources Engineering, Alfa Laval Copenhagen A/S
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Building a Multilevel Modeling Network for Lipid Processing Systems
The world’s fats and oils production has been growing rapidly over the past few decades, exceeding the need for human nutrition. This overproduction combined with the increasing interest among the consumers for healthier food products and bio-fuels, has led the oleo chemical industry to face in the upcoming years major challenges in terms of design and development of better products and more sustainable processes. Although the oleo chemical industry is mature and based on well established processes, the complex systems that lipid compounds form, the lack of accurate predictive models for their physical properties and unit operation models for their processing have limited computer-aided methods and tools for process synthesis, modeling and simulation to be widely used for design, analysis, and optimization of these processes. The world’s fats and oils production has been growing rapidly over the past few decades, exceeding the need for human nutrition. This overproduction combined with the increasing interest among the consumers for healthier food products and bio-fuels, has led the oleo chemical industry to face in the upcoming years major challenges in terms of design and development of better products and more sustainable processes. Although the oleo chemical industry is mature and based on well established processes, the complex systems that lipid compounds form, the lack of accurate predictive models for their physical properties and unit operation models for their processing have limited computer-aided methods and tools for process synthesis, modeling and simulation to be widely used for design, analysis, and optimization of these processes.

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Closed-Loop and Semi Closed-Loop Strategies for Control of Blood Glucose In people with Type 1 Diabetes

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CO2 capture using aqueous ammonia: kinetic study and process simulation
Carbon dioxide capture using aqueous ammonia is a post-combustion technology that has shown a good potential. Therefore this process is studied by measuring the rate of absorption of carbon dioxide by aqueous ammonia and by performing process simulation. The rate of absorption of carbon dioxide by aqueous ammonia solvent has been studied by applying a wetted wall column apparatus. The rate of absorption is crucial regarding the sizing of the absorber columns. The overall mass transfer coefficient has been measured at temperatures from 279 to 304 K for 1 to 10 wt% ammonia solutions at loadings up to 0.6. The results were compared with those found for 30 wt% mono-ethanolamine (MEA) solutions. The capture process was simulated successfully using the simulator Aspen Plus coupled with the extended UNIQUAC thermodynamic model available for the NH3–CO2–H2O system. For this purpose, a user model interface was developed. The heat and electricity requirements were analyzed for a base case configuration, and a preliminary sensitivity analysis was performed on the heat and the electricity requirements and on the ammonia slip from the absorber.

General information
Comparison of Two Methods for Speeding Up Flash Calculations in Compositional Simulations

Flash calculation is the most time consuming part in compositional reservoir simulations and several approaches have been proposed to speed it up. Two recent approaches proposed in the literature are the shadow region method and the Compositional Space Adaptive Tabulation (CSAT) method. The shadow region method reduces the computation time mainly by skipping stability analysis for a large portion of compositions in the single phase region. In the two-phase region, a highly efficient Newton-Raphson algorithm can be employed with initial estimates from the previous step. The CSAT method saves computation time by replacing some of the phase split calculation in the two-phase region with pre-stored flash calculation results. The stored results can be used when the new feed composition is on one of the stored tie lines within a certain tolerance. The number of tie lines stored for comparison and the tolerance set for accepting the feed composition are the key parameters in this method since they will influence the simulation speed and the accuracy of simulation results. Inspired by CSAT, we proposed a Tieline Distance Based Approximation (TDBA) method to get approximate flash results in the twophase region. The method uses the distance to a previous tieline in the same gridblock to decide whether the approximation should be made. Comparison between the shadow region approach and the approximation approach, including CSAT and TDBA, has been made by using a slimtube simulator where the simulation temperature and the simulation pressure are set constant. It is shown that TDBA can significantly improve the flash calculations in the two-phase region.
Distribution of Complex Chemicals in Oil-Water Systems

The deepwater energy sector represents one of the major growth areas of the oil and gas industry today. In order to meet the challenges of hydrate formation, corrosion, scaling and foaming the oil and gas industry uses many chemicals and their use has increased significantly over the years. In order to inhibit gas hydrate formation in subsea pipelines monoethylene glycol (MEG) and methanol are injected in large amounts. It is important to know the distribution of these chemicals in oil and water systems for economical operation of a production facility and to evaluate their impact on marine life. Furthermore, distribution of chemicals is important information for downstream processing of oil and gas. The purpose of this project is the experimental measurement and the thermodynamic modeling of distribution of these complex chemicals in oil-water systems.

Traditionally, distribution of chemicals in oil-water systems is calculated using octanol-water partition coefficients. But experiments carried out by Statoil R & D have shown that octanol-water partition coefficients ($K_{ow}$) do not always mimic oil-water partition coefficients ($K_{oil-water}$) and therefore calculations may not be always correct. In the first phase of this project experimental data on $K_{ow}$, $K_{oil-water}$ and $K_{hw}$ (hexane-water partition coefficients) are collected and investigations were carried out to develop correlations so that $K_{oil-water}$ can be predicted using $K_{ow}$ and $K_{hw}$. However, due to scarcity of experimental data and limited information about the molecular structure of production chemicals the correlation could only be obtained for few families like alcohols, glycols and alkanolamines with varying degree of reliability.

In order to develop a thermodynamic model for the distribution of chemicals in oil-water systems experimental data are required but such data with natural gas-condensate/oil systems are very rare in the literature. In this project experimental work has been carried at Statoil R & D and an experimental method has been established and tested for such measurements. The mutual solubility of two North Sea condensates, MEG and water has been measured in the temperature range of 275-326 K at atmospheric pressure. The detailed composition of condensates is measured by GC analysis and 85 components are identified up to n-nonane and hundreds of ill-defined components in decane plus fraction.

In order to develop a thermodynamic model for the distribution of chemicals in oil-water systems experimental data are required but such data with natural gas-condensate/oil systems are very rare in the literature. In this project experimental work has been carried at Statoil R & D and an experimental method has been established and tested for such measurements. The mutual solubility of two North Sea condensates, MEG and water has been measured in the temperature range of 275-326 K at atmospheric pressure. The detailed composition of condensates is measured by GC analysis and 85 components are identified up to n-nonane and hundreds of ill-defined components in decane plus fraction.

When methanol and MEG are used as gas hydrate inhibitors, the most significant disadvantage, especially for methanol,
is their loss in hydrocarbon phase(s). The successful estimation of inhibitor loss would enable the inhibitors injection optimization as a function of the system parameters such as temperature and water cut. In this project the distribution of water and inhibitors (methanol, MEG) in various phases is modeled using the CPA EoS. The hydrocarbon phase consists of mixture-1 (methane, ethane, n-butane) or mixture-2 (methane, ethane, propane, n-butane, n-heptane, toluene and n-decane). CPA can satisfactorily predict water content in the gas phase of the multicomponent systems containing mixture-1 over a range of temperature and pressure. Similarly the methanol content in gas phase of mixture-1 + water + methanol systems is predicted satisfactorily with accuracy in the range of experimental uncertainty. For VLLE of mixture-2 + water, mixture-2 + MEG + water and mixture-2 + methanol + water systems, the organic phase compositions are satisfactorily predicted whereas modeling results are relatively less satisfactory for vapor phase compositions partially due to uncertainties in the experimental data.

In addition to the multicomponent systems described above, the VLE of the binary system of methane-methanol is also investigated using CPA with satisfactory calculations of methanol content of liquid phase using a single temperature independent kij over a range of temperature and pressure. The methanol content in the gas phase is satisfactorily correlated at higher temperatures and lower pressures using the same kij but deviations from experimental data are observed at lower temperatures and higher pressures. In order to extend CPA to reservoir fluids it is of interest to investigate the LLE of binary systems of hydrocarbons and water. In this work CPA is also applied to alkaline + water and alkylbenzene + water systems to obtain binary interaction parameters and cross-association volumes respectively.

Finally, CPA has been extended to reservoir-fluid + MEG and reservoir-fluid + MEG + water systems. The reservoir fluid consists of three condensates and two oils from the gas fields in the North Sea. The mutual solubility of condensates and MEG is satisfactorily correlated using a single, average and temperature independent kij for all MEG-HC pairs. Similarly the mutual solubility of condensate/oil, MEG and water is predicted satisfactorily using the same average kij for MEG-HC pairs and water-HC kij from a generalized correlation as a function of carbon number. The experimental trends in mutual solubility as a function of temperature and MEG content in polar phase are predicted satisfactorily which are correct in order of magnitude according to the industrial requirements.
Economic MPC for Power Management in the Smart Grid
To increase the amount of green energy (e.g. solar and wind) significantly a new intelligent electrical infrastructure is needed. We must not only control the production of electricity but also the consumption in an efficient and proactive manner. This future intelligent grid is in Europe known as the SmartGrid. In this paper we demonstrate the use of Economic Model Predictive Control to operate a portfolio of power generators and consumers such that the cost of producing the required power is minimized. With conventional coal and gas fired power generators representing the controllable power production and a significant share of renewable energy, such as parks of wind turbines, representing the uncontrollable power generators we have demonstrated how the addition of controllable consumers, such as large cold rooms or supermarkets with a thermal capacity, can infuse the desired flexibility of the grid for utilization of more green energy and also lower the total cost. We formulate the supply-demand constraint as a probabilistic constraint, thereby robustifying the solution against uncertainties in power demand. We use small conceptual examples for simulations.

General information
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Organisations: Scientific Computing, Department of Informatics and Mathematical Modeling, Center for Energy Resources Engineering, DONG Energy A/S
Authors: Hovgaard, T. G. (Intern), Edlund, K. (Ekstern), Jørgensen, J. B. (Intern)
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Elastic moduli of sandstones saturated with a range of pore fluids correlated with kinematic viscosity and frequency ratio is a common need in exploration geophysics. Such modeling commonly involves formulation of a set of frame parameters which are then perturbed by the presence of a fluid in the pores. Frame parameters are extracted from laboratory measurements on dry samples meaning samples saturated only with air. The purpose of this study is to investigate if frame parameters can be extracted from air saturated measurements in sandstones, because earlier studies have shown that air may have a non-negligible effect on carbonates due to the high kinematic viscosity of air (Fabricius et al., 2010).

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Energy Efficient Refrigeration and Flexible Power Consumption in a Smart Grid

Refrigeration and heating systems consume substantial amounts of energy worldwide. However, due to the thermal capacity there is a potential for storing “coldness” or heat in the system. This feature allows for implementation of different load shifting and shedding strategies in order to optimize the operation energywise, but without compromising the original cooling and indoor climate quality. In this work we investigate the potential of such a strategy and its ability to significantly lower the cost related to operating systems such as supermarket refrigeration and heat pumps for residential houses. With modern Economic Model Predictive Control (MPC) methods we make use of weather forecasts and predictions of varying electricity prices to apply more load to the system when the thermodynamic cycle is most efficient, and to consume larger shares of the electricity when the demand and thereby the prices are low. The ability to adjust power consumption according to the demands on the power grid is a highly wanted feature in a future Smart Grid. Efficient utilization of greater amounts of renewable energy calls for solutions to control the power consumption such that it increases when an energy surplus is available and decreases when there is a shortage. This should happen almost instantly to accommodate intermittent energy sources as e.g. wind turbines. We expect our power management solution to render systems with thermal storage capabilities suitable for flexible power consumption. The aggregation of several units will contribute significantly to the shedding of total electricity demand. Using small case studies we demonstrate the potential for utilizing daily variations to deliver a power efficient cooling or heating and for the implementation of Virtual Power Plants in Smart Grid scenarios.

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Organisations: Scientific Computing, Department of Informatics and Mathematical Modeling, Center for Energy Resources Engineering, Danfoss A/S
Authors: Hovgaard, T. G. (Intern), Halvgaard, R. (Intern), Larsen, L. F. (Ekstern), Jørgensen, J. B. (Intern)
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Experimental measurement and modeling of the rate of absorption of carbon dioxide by aqueous ammonia

In this work, the rate of absorption of carbon dioxide by aqueous ammonia solvent has been studied by applying a newly built wetted wall column. The absorption rate in aqueous ammonia was measured at temperatures from 279 to 304K for 1 to 10wt% aqueous ammonia with loadings varying from 0 to 0.8molCO2/molNH3. The absorption rate in 30wt% aqueous mono-ethanolamine (MEA) was measured at 294 and 314K with loadings varying from 0 to 0.4 as comparison. It was found that at 304K, the rate of absorption of carbon dioxide by 10wt% NH3 solvent was comparable to the rates for 30wt% MEA at 294 and 314K (a typical absorption temperature for this process). The absorption rate using ammonia was however significantly lower at temperatures of 294K and lower as applied in the Chilled Ammonia Process. However, at these low temperatures, the rate of absorption in ammonia has only a small temperature dependency. The rate of absorption decreases strongly with decreasing ammonia concentrations and increasing CO2 loadings. The rate of absorption of carbon dioxide by aqueous ammonia solvent was modeled using the measurements of the unloaded solutions and the zwitter-ion mechanism. The model could successfully predict the experimental measurements of the absorption rate of CO2 in loaded ammonia solutions.

General information
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Organisations: CERE – Center for Energy Ressources Engineering, Department of Chemical and Biochemical Engineering, Department of Chemistry, Center for Energy Resources Engineering, DONG Energy A/S
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Filtration in Porous Media: Influential Parameters and Comparison with Experiments

There is a considerable and ongoing effort aimed at understanding the transport and the deposition of suspended particles in porous media, especially non-Fickian transport and non-exponential deposition of particles. In this work, the influential parameters in filtration models are studied to understand their effects on the non-Fickian transport and the non-exponential deposition. The filtration models are validated by the comparisons between the modelling results and the experimental data. The elliptic equation with distributed filtration coefficients may be applied to model non-Fickian transport and hyperexponential deposition. The filtration model accounting for the migration of surface associated particles may be applied for non-monotonic deposition.

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Organisations: CERE – Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Finite Horizon MPC for Systems in Innovation Form
System identification and model predictive control have largely developed as two separate disciplines. Nevertheless, the major part of industrial MPC commissioning is generation of data and identification of models. In this contribution we attempt to bridge this gap by contributing some of the missing links. Input-output models (FIR, ARX, ARMAX, Box-Jenkins) as well as subspace models can be represented as state space models in innovation form. These models have correlated process and measurement noise. The correct LQG control law for systems with correlated process and measurement noise is not well known. We provide the correct finite-horizon LQG controller for this system and use this to develop a state space representation of the closed-loop system. This representation is used for closed-loop frequency and covariance analysis. These measures are used in tuning of the unconstrained and constrained MPC. We demonstrate our results on a simulated industrial furnace.

Flexible and Cost Efficient Power Consumption using Economic MPC: A Supermarket Refrigeration Benchmark
Supermarket refrigeration consumes substantial amounts of energy. However due to the thermal capacity in the refrigerated goods parts of the delivered cooling capacity can be shifted in time without deteriorating the food quality. In this paper we introduce a novel economic optimizing MPC scheme that reduces operation costs by utilizing the thermal storage capabilities. In the study we specifically address advantages coming from daily variations in outdoor temperature and electricity prices but other aims such as peak load reduction are also considered. An important contribution of this paper is also the formulation of a new cost function for our proposed power management. Hereby the refrigeration system is enabled to contribute with ancillary services to the balancing power market. Since significant amounts of regulating power is needed for a higher penetration of intermittent renewable energy sources such as wind turbines this feature is in high demand in a future intelligent power grid (Smart Grid). Our perspective is seen from the refrigeration system but as it is demonstrated the involvement in the balancing market can be economically beneficial for the system itself while delivering crucial services to the Smart Grid. We simulate the system using models validated against data from real supermarkets as well as weather data and spot and regulating power prices from the Nordic power market.
Hierarchical model-based predictive control of a power plant portfolio

One of the main difficulties in large-scale implementation of renewable energy in existing power systems is that the production from renewable sources is difficult to predict and control. For this reason, fast and efficient control of controllable power producing units – so-called “portfolio control” – becomes increasingly important as the ratio of renewable energy in a power system grows. As a consequence, tomorrow’s “smart grids” require highly flexible and scalable control systems compared to conventional power systems. This paper proposes a hierarchical model-based predictive control design for power system portfolio control, which aims specifically at meeting these demands. The design involves a two-layer hierarchical structure with clearly defined interfaces that facilitate an object-oriented implementation approach. The same hierarchical structure is reflected in the underlying optimisation problem, which is solved using Dantzig–Wolfe decomposition. This decomposition yields improved computational efficiency and better scalability compared to centralised methods. The proposed control scheme is compared to an existing, state-of-the-art portfolio control system (operated by DONG Energy in Western Denmark) via simulations on a real-world scenario. Despite limited tuning, the new controller shows improvements in terms of ability to track reference production as well as economic performance.

General information
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Publication information
High kinematic viscosity of air may cause dry clay to be stiffer than water saturated clay

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Authors: Fabricius, I. L. (Intern)
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High-Temperature Release of SO2 from Calcined Cement Raw Materials
During combustion of alternative fuels in the material inlet end of cement rotary kilns, local reducing conditions may occur and cause reductive decomposition of sulfates from calcined cement raw materials. Decomposition of sulfates is problematic because it increases the gas-phase SO2 concentration, which may cause deposit formation in the kiln system. In this study, the release of sulfur from calcined cement raw materials under both oxidizing and reducing conditions is investigated. The investigations include thermodynamic equilibrium calculations in the temperature interval of 800–1500 °C and experiments in a tube furnace reactor in the temperature interval of 900–1100 °C. The investigated conditions resemble actual conditions in the material inlet end of cement rotary kilns. It was found that the sulfates CaSO4, K2SO4, and Na2SO4 were all stable under oxidizing conditions but began to decompose under reducing conditions. Particularly, CaSO4 was sensitive to reducing conditions. The sulfur release was most significant if the gas atmosphere frequently shifted between oxidizing and reducing conditions. An increasing temperature from 900 to 1100 °C under alternating oxidizing and reducing conditions was also observed to increase the sulfur release from the calcined raw materials by a factor of 3, from 14 to 48%.

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BFI (2014): BFI-level 2
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Impact of supercritical CO2 injection on petrophysical and rock mechanics properties of chalk: an experimental study on chalk from South Arne field, North Sea.

Changes in chalk due to EOR by injecting supercritical CO2 (CO2-EOR) can ideally be predicted by applying geophysical methods designed from laboratory-determined petrophysical and rock mechanics properties. A series of petrophysical and rock mechanics tests were performed on Ekofisk Formation and Tor Formation chalk of the South Arne field to reveal the changes in petrophysical and rock mechanics properties of chalk due to the injection of CO2 at supercritical state. An increase in porosity and decrease in specific surface was observed due to injection of supercritical CO2. This indicates that a reaction between CO2 enriched water and particles takes place which smoothenes the particle surface. Accordingly, partial increase in permeability was also noticed. An effect is also observed from the decrease in pore-space stiffness, calculated from sonic velocity. No significant effect on wettability as indicated by NMR T2 relaxation time was observed. Rock mechanics testing indicates that in 30% porosity chalk from the South Arne field, injection of supercritical CO2 has no significant effect on shear strength and compaction properties, while there is probably a slight decrease in stiffness properties. For both the Tor Formation and Ekofisk Formation, flooding with CO2 after waterflooding does not seem to affect the shear strength parameters. For the Tor Formation, the elastic deformation parameters seem to be reduced after CO2 injection. In contrast, the effect on the elastic moduli in Ekofisk Formation is insignificant. The time dependent properties for both Tor Formation and Ekofisk Formation do not seem to be affected by CO2 flooding in the relevant stress regime. Generally, the change in both petrophysical and rock-mechanics properties is insignificant in Ekofisk Formation, compared to the changes in Tor Formation, most probably due to the very little contact cement in Ekofisk Formation chalk. Time-lapse monitoring strategies may be required during a CO2-EOR process for the measurement of changes in reservoir properties that may cause deformation of and leakage from a reservoir. Results of this study will provide data for designing future monitoring strategies based on 4D seismic.
Induced migration of fines during waterflooding in communicating layer-cake reservoirs
The effects of fines migration induced by injection of water with a different salinity than the reservoir brine are incorporated into the upscaling model for waterflooding in a layer cake reservoir with good communication between the layers. Mobilization and re-capturing of the reservoir fines may give rise to reduction of the permeability in water swept zones, which subsequently leads to the diversion of water flow from the initially more permeable layers to the less permeable ones. As a result, the displacement is more even, the water cut at the producer is decreased, and the oil recovery is increased. On the other hand, more energy for the pressure drop is required to maintain a constant flow rate. These effects are studied within a new upscaling model developed previously (Zhang et al., 2011). In a communicating layer cake reservoir, higher end-point mobility ratio (water to oil) leads to more crossflow between layers and lowers the water sweep efficiency. However, this ratio facilitates the fluid diversion caused by the fines migration, leading to a more efficient enhanced oil recovery. The positive contribution from the mobility ratio to the increased oil recovery due to fines migration seems to be limited.
The objective of this study was to discuss the influence of pore fluid on elastic properties of greensand. Gassmann’s equations generally work at low frequency and do not take into consideration the fluid related dispersion. In some cases Biot’s theory is used to describe the fluid related dispersion. However, Biot’s theory does not fully explain the frequency dispersion of sedimentary rocks. Greensands are composed of a mixture of quartz and micro-porous glauconite grains. In greensand, it is possible that the contrast between flow in macro-pores and micro-pores within glauconites gives rise to a local stiffening pressure gradient in the fluid. Then fluid flow in greensand could then be described as a kind of squirt flow. Greensand data from the North Nini filed was included in this study. Gassmann’s, Biot’s and squirt models were used to discuss the influence of pore fluid on elastic moduli. Biot’s critical frequency and NMR (nuclear magnetic resonance) T2 spectrum were combined to describe the differences in fluid flow within macro-pores and within micro-pores. NMR data show that Biot’s flow should occur only in large pores in the greensand while, Biot’s flow should not occur in micro-pores. Differences of fluid flow in macro-pores and micro-pores pores are described as high frequency squirt flow in greensand.

**Influence of pore fluid and frequency on elastic properties of greensand as interpreted using NMR data**

**General information**

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Organisations: Department of Civil Engineering, Section for Geotechnics and Geology, Center for Energy Resources Engineering, Stanford University
Insulin Administration for People with Type 1 diabetes

In this paper, we apply model predictive control (MPC) for control of blood glucose in people with type 1 diabetes. The two first control strategies are based on nonlinear model predictive control (NMPC). The first control strategy is based on meal announcement in advance, while the second one considers meal announcement at mealtimes only. They give a quantitative upper bound on the achievable control performance. The third control strategy is a feedforward-feedback control strategy. This strategy uses a time-varying setpoint to reduce the risk of hypoglycemia. The feedback controller computes the optimal basal insulin infusion rate. The feedforward controller consists of a bolus calculator. It computes the optimal bolus, along with the time-varying glucose setpoint. We test these three strategies on a virtual patient with type 1 diabetes. The numerical results demonstrate the robustness of the last control strategy with respect to changes in the model parameters and incorrect meal announcement.

Integrated seismic analysis of the Chalk Group in eastern Denmark—Implications for estimates of maximum palaeo-burial in southwest Scandinavia

The origin of the topography of southwest Scandinavia is subject to discussion. Analysis of borehole seismic velocity has formed the basis for interpretation of several hundred metres of Neogene uplift in parts of Denmark. Here, refraction seismic data constrain a 7.5km long P-wave velocity model of the Chalk Group below the Stevns peninsula, eastern part of the Danish Basin. The model contains four layers in the ~860m thick Chalk Group with mean velocities of 2.2km/s, 2.4km/s, 3.1km/s, and 3.9–4.3km/s. Sonic and gamma wireline log data from two cored boreholes represent the upper ~450m of the Chalk Group. The sonic velocities are consistent with the overall seismic layering, although they show additional fine-scale layering. Integration of gamma and sonic log with porosity data shows that seismic velocity is sensitive to clay content. In intervals near boundaries of the refraction model, moderate increases in clay content correlate with reduction of porosity and increase in velocity. Higher clay contents do not further increase velocity. The reduction of porosity and increase in velocity are interpreted as clay causing increased pressure dissolution and cementation. The interpreted velocities are systematically higher than values of a chalk velocity curve determined in previous studies, and it is estimated that a significant part of the velocity anomaly may be explained by the presence of clay. The remaining
velocity anomaly can be explained by 450–500m palaeo-burial of the Chalk Group. The burial anomaly will be overestimated by ~150–200m if the analysis is based on the average Chalk Group velocity and clay content is disregarded. Burial anomaly values of ~450–600m result if the strongest velocity contrast at ~600–650m depth is interpreted to be a result of diagenetic effects, consistent with the clay-corrected estimates within uncertainty.

**General information**

State: Published
Organisations: Scientific Computing, Department of Informatics and Mathematical Modeling, Center for Energy Resources Engineering, Aarhus University, University of Copenhagen
Authors: Nielsen, L. (Ekstern), Boldreel, L. O. (Ekstern), Hansen, T. M. (Intern), Lykke-Andersen, H. (Ekstern), Stemmerik, L. (Ekstern), Suryk, F. (Ekstern), Thybo, H. (Ekstern)
Pages: 14-26
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Main Research Area: Technical/natural sciences

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Scopus rating (2016): CiteScore 2.96 SJR 1.706 SNIP 1.35
Web of Science (2016): Indexed yes
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BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.769 SNIP 1.425 CiteScore 2.91
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.817 SNIP 1.598 CiteScore 3.18
ISI indexed (2013): ISI indexed yes
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BFI (2012): BFI-level 1
Scopus rating (2012): SJR 2.012 SNIP 1.504 CiteScore 2.79
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 2.018 SNIP 1.295 CiteScore 2.48
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
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BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.435 SNIP 1.377
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 1.478 SNIP 1.206
Scopus rating (2007): SJR 1.602 SNIP 1.342
Scopus rating (2006): SJR 1.557 SNIP 1.422
Scopus rating (2005): SJR 1.9 SNIP 1.448
Scopus rating (2004): SJR 1.763 SNIP 1.42
Scopus rating (2003): SJR 1.676 SNIP 1.418
Scopus rating (2002): SJR 1.749 SNIP 1.333
Scopus rating (2001): SJR 1.674 SNIP 1.214
Intramolecular Association within the SAFT Framework

A general theory for modelling intramolecular association within the SAFT framework is proposed. Sear and Jackson [Phys. Rev. E. 50 (1), 386 (1994)] and Ghonasgi and Chapman [J. Chem. Phys. 102 (6), 2585 (1995)] have previously extended SAFT to include intramolecular association for chains with two sites. We show that the resulting equations from the two approaches are equivalent, and use their work as a basis for developing a new general theory. The approach used by Ghonasgi and Chapman is based on mass balances and an infinite dilution result and provides the equations needed to determine the contribution to the Helmholtz free energy from association (inter- as well as intramolecularly) at equilibrium. Sear and Jackson rederived the contribution to the Helmholtz free energy from association from the theory by Wertheim [J. Stat. Phys. 42 (3–4), 459 (1986)] with inclusion of intramolecular association, and using this approach we obtain an expression for the Helmholtz free energy that is valid also at non-equilibrium states (with respect to hydrogen bonds), which is very useful when calculating derivatives.

General information
State: Published
Organisations: CERE – Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering, Rice University
Authors: Avlund, A. S. (Intern), Kontogeorgis, G. (Intern), Chapman, W. G. (Ekstern)
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Main Research Area: Technical/natural sciences

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Web of Science (2017): Indexed yes
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Scopus rating (2016): CiteScore 1.65 SJR 0.833 SNIP 0.729
Web of Science (2016): Indexed yes
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BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.697 SNIP 0.667 CiteScore 1.48
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BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.678 SNIP 0.715 CiteScore 1.58
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.801 SNIP 0.738 CiteScore 1.62
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.824 SNIP 0.829 CiteScore 1.67
Lipid Processing Technology: Building a Multilevel Modeling Network

Over the past few decades, the world’s fats and oils production has been growing rapidly, far beyond the need for human nutrition. This overproduction combined with the growing consumer preferences for healthier food products and the interest in bio-fuels, has led the oleo chemical industry to face in the upcoming years major challenges in terms of design and development of better products and more sustainable processes. Although the oleo chemical industry is mature and based on well established processes, the complex systems that lipid compounds form, the lack of accurate predictive models for their physical properties and unit operation models for their processing have limited computeraided methods and tools for process synthesis, modeling and simulation to be widely used for design, analysis, and optimization of these processes. In consequence, the aim of this work is to present the development of a computer aided multilevel modeling network consisting a collection of new and adopted models, methods and tools for the systematic design and analysis of processes employing lipid technology. This is achieved by decomposing the problem into four levels of modeling: 1. pure component properties; 2. mixtures and phase behavior; 3. unit operations; and 4. process synthesis and design. The methods and tools in each level include: For the first level, a lipid-database of collected experimental data from the open literature, confidential data from industry and generated data from validated predictive property models; as well as modeling tools for fast adoption analysis of property prediction models. In the second level, phase behaviors (VLE, LLE and SLE) of relevant lipid mixtures are predicted using the UNIFAC-CI model where missing group interaction parameters are predicted using the GCPPlus approach (connectivity index). A master parameter table is prepared for this purpose. In the third level, a detailed computer aided model analysis of unit operations encountered in oleo chemical industry (eg. Transesterification, Hydrogenation, Interesterification etc.), optimal design, operation and control of these unit operations with respect to performance parameters such as minimum total cost, product yield improvement, operability etc., and process intensification for the retrofit of existing biofuel plants. In the fourth level the information and models developed are used as building blocks in the development of methods and tools for computer-aided synthesis and design of process flowsheets (CAFD), feasibility assessment and comparison of the alternative flowsheets at their optimal operating points and optimization of the selected alternative with respect to cost and sustainability indicators.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, CERE – Center for Energy Ressources Engineering, Center for Energy Resources Engineering, Alfa Laval Copenhagen A/S
Authors: Diaz Tovar, C. A. (Intern), Mustaffa, A. A. (Intern), Hukkerikar, A. (Intern), Quaglia, A. (Intern), Sin, G. (Intern), Kontogeorgis, G. (Intern), Sarup, B. (Ekstern), Gani, R. (Intern)
Measurement and modeling of CO2 solubility in NaCl brine and CO2–saturated NaCl brine density

Phase equilibrium for CO2–NaCl brine is of general interest to many scientific disciplines and technical areas. The system is particularly important to CO2 sequestration in deep saline aquifers and CO2 enhanced oil recovery, two techniques discussed intensively in recent years due to the concerns over climate change and energy security. This work is an experimental and modeling study of two fundamental properties in high pressure CO2–NaCl brine equilibrium, i.e., CO2 solubility in NaCl brine and CO2–saturated NaCl brine density. A literature review of the available data was presented first to illustrate the necessity of experimental measurements of the two properties at high pressures. An experimental method for measuring high pressure CO2 solubility in NaCl brine was then developed. With the method, CO2 solubilities in 0, 1, and 5m NaCl brines were measured at 323, 373, and 413K from 5 to 40MPa. The corresponding density data at the same conditions were also measured. For solubility, two models used in the Eclipse simulator were tested: the correlations of Chang et al. and the Søreide and Whitson equation of state (EoS) model. The latter model was modified to improve its performance for high salinity brine. In the density modeling, the correlations of Chang et al., Garcia's correlation, and five different EoS models were tested. Among these models, Garcia's correlation and the ePC-SAFT EoS generally give satisfactory agreement with the experimental measurements. An analysis was also made to show that dissolution of CO2 increases the brine density only if the apparent mass density of CO2 in brine is higher than the brine density at the same conditions.
Measurement of liquid-liquid equilibria for condensate + glycol and condensate + glycol + water systems

Today's oil and gas production requires the application of various chemicals in large amounts. To evaluate the effects of those chemicals on the environment, it is of crucial importance to know how much of the chemicals are discharged via produced water and how much is dissolved in the crude oil. The ultimate objective of this work is to develop a predictive thermodynamic model for the mutual solubility of oil, water, and polar chemicals. But for the development and validation of the model, experimental data are required. This work presents new experimental liquid-liquid equilibrium (LLE) data for 1,2-ethanediol (MEG) + condensate and MEG + water + condensate systems at temperatures from (275 to 323) K at atmospheric pressure. The condensate used in this work is a stabilized natural gas condensate from an offshore field in the North Sea. Compositional analysis of the natural gas condensate was carried out by gas chromatography, and detailed separation of individual condensate's components has been carried out. Approximately 85 peaks eluting before nonane were identified by their retention time. Peak areas were converted to mass fraction using 1-heptene as an internal standard. The components were divided into boiling range groups from hexane to nonane. Paraffinic (P), naphthenic (N), and aromatic (A) distributions were obtained for the boiling point fractions up to nonane. The average molar mass and the overall density of the condensate were measured experimentally. For the mutual solubility of MEG and condensate, approximately 72 component peaks could be detected up to nonane and many components from decane plus carbon fraction. Their solubility was quantified, and the sum was reported as solubility of condensate in MEG. A similar procedure was adopted for the MEG, condensate, and water system, but because of the presence of water, the solubility of condensate in the polar phase decreases, and some of the components were not detectable. © 2011 American Chemical Society.

General information

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Organisations: CERE – Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, Department of Chemistry, Center for Energy Resources Engineering, StatOil ASA
Authors: Riaz, M. (Intern), Kontogeorgis, G. (Intern), Stenby, E. H. (Intern), Yan, W. (Intern), Haugum, T. (Ekstern), Christensen, K. O. (Ekstern), Lekken, T. V. (Ekstern), Solbraa, E. (Ekstern)
Pages: 4342-4351
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Web of Science (2017): Indexed Yes
Modeling of phase equilibria with CPA using the homomorph approach

For association models, like CPA and SAFT, a classical approach is often used for estimating pure-compound and mixture parameters. According to this approach, the pure-compound parameters are estimated from vapor pressure and liquid density data. Then, the binary interaction parameters, kij, are estimated from binary systems; one binary interaction parameter per system. No additional mixing rules are needed for cross-associating systems, but combining rules are required, e.g. the Elliott rule or the so-called CR-1 rule. There is a very large class of mixtures, e.g. water or glycols with aromatic hydrocarbons, chloroform–acetone, esters–water, CO2–water, etc., which are classified as "solvating" or "induced associating". The classical approach cannot be used and the cross-association interactions are difficult to be estimated a priori since usually no appropriate experimental data exist, while the aforementioned combining rules cannot capture the physical meaning of such interactions (as at least one of the compounds is non-self-associating).

Consequently, very often one or more of the interaction parameters are optimized to experimental mixture data. For example, in the case of the CPA EoS, two interaction parameters are often used for solvating systems; one for the physical part (kij) and one for the association part (βcross). This limits the predictive capabilities and possibilities of generalization of the model. In this work we present an approach to reduce the number of adjustable parameters in CPA for solvating systems. The so-called homomorph approach will be used, according to which the kij parameter can be obtained from a corresponding system (homomorph) which has similar physical interactions as the solvating system studied. This leaves only one adjustable parameter for solvating mixtures, the cross-association volume (βcross). It is shown that the homomorph approach can be used with success for mixtures of water and glycols with aromatic hydrocarbons as well as for mixtures of acid gases (CO2, H2S) with alcohols and water. The homomorph approach is less satisfactory for mixtures with fluorocarbons as well as for aqueous mixtures with ethers and esters. In these cases, CPA can correlate liquid–liquid equilibria for solvating systems using two adjustable parameters. The capabilities and limitations of the homomorph approach are discussed.
Modeling phase equilibria for acid gas mixtures using the CPA equation of state. Part II: Binary mixtures with CO2

In Part I of this series of articles, the study of H2S mixtures has been presented with CPA. In this study the phase behavior of CO2 containing mixtures is modeled. Binary mixtures with water, alcohols, glycols and hydrocarbons are investigated. Both phase equilibria (vapor–liquid and liquid–liquid) and densities are considered for the mixtures involved. Different approaches for modeling pure CO2 and mixtures are compared. CO2 is modeled as non self-associating fluid, or as self-associating component having two, three and four association sites. Moreover, when mixtures of CO2 with polar compounds (water, alcohols and glycols) are considered, the importance of cross-association is investigated. The cross-association is accounted for either via combining rules or using a cross-solvation energy obtained from experimental spectroscopic or calorimetric data or from ab initio calculations. In both cases two adjustable parameters are used when solvation is explicitly accounted for. The performance of CPA using the various modeling approaches for CO2 and its interactions is presented and discussed, comparatively to various recent published investigations. It is shown that overall very good correlation is obtained for binary mixtures of CO2 and water or alcohols when the solvation between CO2 and the polar compound is explicitly accounted for, whereas the model is less satisfactory when CO2 is treated as self-associating compound.

General information
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Organisations: CERE – Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, Department of Chemistry, Center for Energy Resources Engineering
Model Predictive Control based on Stochastic Dynamic Building Models

**General information**
State: Published
Organisations: Scientific Computing, Department of Informatics and Mathematical Modeling, Center for Energy Resources Engineering
Authors: Halvgaard, R. (Intern)
Publication date: 2011

**Publication information**
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Main Research Area: Technical/natural sciences
Links: http://www.dynastee.info/home.php
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Publication: Research › Sound/Visual production (digital) – Annual report year: 2011

Model predictive control for plant-wide control of a reactor-separation-recycle system

**General information**
State: Published
Organisations: CHEC Research Centre, Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Scientific Computing, Department of Informatics and Mathematical Modeling, Center for Energy Resources Engineering
Authors: Bialas, D. J. (Intern), Huusom, J. K. (Intern), Jørgensen, J. B. (Intern), Sin, G. (Intern)
Publication date: 2011
Main Research Area: Technical/natural sciences
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Publication: Research › Poster – Annual report year: 2011

New Cross-linkers for PDMS Networks

**General information**
State: Published
Organisations: Department of Chemical and Biochemical Engineering, The Danish Polymer Centre, Center for Energy Resources Engineering
Authors: Bahrt, F. (Intern), Daugaard, A. E. (Intern), Hvilsted, S. (Intern), Skov, A. L. (Intern)
Number of pages: 1
Publication date: 2011
Main Research Area: Technical/natural sciences
Electronic versions:
NMPC for Oil Reservoir Production Optimization

In this paper, we use nonlinear model predictive control (NMPC) to maximize secondary oil recovery from an oil reservoir by controlling two-phase subsurface porous flow using adjustable down-hole control valves. The resulting optimal control problem is nonlinear and large-scale. We solve this problem numerically using a single shooting sequential quadratic programming (SQP) based optimization method. Explicit singly diagonally implicit Runge-Kutta (ESDIRK) methods are used for integration of the stiff system of differential equations describing the two-phase flow, and the adjoint method is used for sensitivity computations. We report computational experiences and oil recovery improvements for a standard test case.

Noise Modelling and MPC Tuning for Systems with Infrequent Step Disturbances

In this paper, an offset-free SISO MPC implementation based on an ARX model of the system dynamics is investigated. Special emphasis is directed to achieving good closed loop performance for systems which may be step wised perturbed by a sustained, unmeasured disturbance. Hence a noise model which expresses the behaviour of this non-stationary noise process is sought. Tuning of the ARX-based MPC implementation is discussed and illustrated in a simulation example. Guidelines for tuning of the free parameters are presented.
Noise Modelling and MPC Tuning for Systems with Infrequent Step Disturbances

In this paper, an offset-free SISO MPC implementation based on an ARX model of the system dynamics is investigated. Special emphasis is directed to achieving good closed loop performance for systems which may be step wisdom perturbed by a sustained, unmeasured disturbance. Hence a noise model which expresses the behaviour of this non-stationary noise process is sought. Tuning of the ARX-based MPC implementation is discussed and illustrated in a simulation example. Guidelines for tuning of the free parameters are presented.

General information
State: Published
Organisations: Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Department of Informatics and Mathematical Modeling, Mathematical Statistics, Scientific Computing
Authors: Huusom, J. K. (Intern), Poulsen, N. K. (Intern), Jørgensen, S. B. (Intern), Jørgensen, J. B. (Intern)
Publication date: 2011
Event: Abstract from 18th World Congress of the International Federation of Automatic Control, Milano, Italy.
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 282995
Publication: Research - peer-review › Article in proceedings – Annual report year: 2011

Oil Reservoir Production Optimization using Optimal Control

Practical oil reservoir management involves solution of large-scale constrained optimal control problems. In this paper we present a numerical method for solution of large-scale constrained optimal control problems. The method is a single-shooting method that computes the gradients using the adjoint method. We use an Explicit Singly Diagonally Implicit Runge-Kutta (ESDIRK) method for the integration and a quasi-Newton Sequential Quadratic Programming (SQP) algorithm for the constrained optimization. We use this algorithm in a numerical case study to optimize the production of oil from an oil reservoir using water flooding and smart well technology. Compared to the uncontrolled case, the optimal operation increases the Net Present Value of the oil field by 10%.

General information
State: Published
Organisations: Department of Informatics and Mathematical Modeling, Scientific Computing, Department of Chemistry, Center for Energy Resources Engineering
Authors: Völcker, C. (Intern), Jørgensen, J. B. (Intern), Stenby, E. H. (Intern)
Pages: 7937-7943
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Main Research Area: Technical/natural sciences
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ISSN (Print): 0743-1546
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BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 0.68
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BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 0.66
ISI indexed (2012): ISI indexed no
BFI (2011): BFI-level 1
Compositional reservoir simulation uses almost exclusively cubic equations of state (EoS) such as the SRK EoS and the PR EoS. This is in contrast with process simulation in the downstream industry where more recent and advanced thermodynamic models are quickly adopted. Many of these models are non-cubic EoS, such as the PC-SAFT EoS. A major reason for the use of the conventional cubic EoS in reservoir simulation is the concern over computation time. Flash computation is the most time consuming part in compositional reservoir simulation, and the extra complexity of the non-cubic EoS may significantly increase the time consumption. In addition to this, the non-cubic EoS also needs a C7+ characterization. The main advantage of the non-cubic EoS is that it provides for a more accurate description of fluid properties, and it is therefore of interest to investigate the computational aspects of using such models.

In this work we test the feasibility of applying a non-cubic EoS to reservoir simulation, using a slimtube simulator to simulate multicomponent gas injection using both the traditional SRK EoS and the non-cubic PC-SAFT EoS. Computation times for both models were compared. In addition, C7+ characterization for PC-SAFT and the performance of PC-SAFT in PVT modeling are also addressed.

**On Implementing a Homogeneous Interior-Point Algorithm for Nonsymmetric Conic Optimization**

Based on earlier work by Nesterov, an implementation of a homogeneous infeasible-start interior-point algorithm for solving nonsymmetric conic optimization problems is presented. Starting each iteration from (the vicinity of) the central path, the method computes (nearly) primal-dual symmetric approximate tangent directions followed by a purely primal centering procedure to locate the next central primal-dual point. Features of the algorithm include that it makes use only of the primal barrier function, that it is able to detect infeasibilities in the problem and that no phase-I method is needed. The method further employs quasi-Newton updating both to generate (pseudo) higher order directions and to reduce the number of factorizations needed in the centering process while still retaining the ability to exploit sparsity. Extensive and promising computational results are presented for the p-cone problem, the facility location problem, entropy problems and geometric programs; all formulated as nonsymmetric conic optimization problems.
Permeability prediction in chalks

The velocity of elastic waves is the primary datum available for acquiring information about subsurface characteristics such as lithology and porosity. Cheap and quick (spatial coverage, ease of measurement) information of permeability can be achieved, if sonic velocity is used for permeability prediction, so we have investigated the use of velocity data to predict permeability. The compressional velocity from wireline logs and core plugs of the chalk reservoir in the South Arne field, North Sea, has been used for this study. We compared various methods of permeability prediction from velocities. The relationships between permeability and porosity from core data were first examined using Kozeny’s equation. The data were analyzed for any correlations to the specific surface of the grain, $S_g$, and to the hydraulic property defined as the flow zone indicator (FZI). These two methods use two different approaches to enhance permeability prediction from Kozeny’s equation. The FZI is based on a concept of a tortuous flow path in a granular bed. The $S_g$ concept considers the pore space that is exposed to fluid flow and models permeability resulting from effective flow parallel to pressure drop. The porosity-permeability relationships were replaced by relationships between velocity of elastic waves and permeability using laboratory data, and the relationships were then applied to well-log data. We found that the permeability prediction in chalk and possibly other sediments with large surface areas could be improved significantly using the effective specific surface as the fluid-flow concept. The FZI unit is appropriate for highly permeable sedimentary rocks such as sandstones and limestones that have small surface areas.

General information
State: Published
Organisations: Section for Geotechnics and Geology, Department of Civil Engineering, Center for Energy Resources Engineering, Colorado School of Mines
Authors: Alam, M. M. (Intern), Fabricius, I. L. (Intern), Prasad, M. (Ekstern)
Pages: 1991-2014
Publication date: 2011
Main Research Area: Technical/natural sciences

Publication information
Petrophysical properties of greensand as predicted from NMR measurements

ABSTRACT: Nuclear magnetic resonance (NMR) is a useful tool in reservoir evaluation. The objective of this study is to predict petrophysical properties from NMR T2 distributions. A series of laboratory experiments including core analysis, capillary pressure measurements, NMR T2 measurements and image analysis were carried out on sixteen greensand samples from two formations in the Nini field of the North Sea. Hermod Formation is weakly cemented, whereas Ty Formation is characterized by microcrystalline quartz cement. The surface area measured by the BET method and the NMR derived surface relaxivity are associated with the micro-porous glauconite grains. The effective specific surface area as calculated from Kozeny's equation and as derived from petrographic image analysis of backscattered electron
micrograph's (BSE), as well as the estimated effective surface relaxivity, is associated with macro-pores. Permeability may be predicted from NMR by using Kozeny's equation when surface relaxivity is known. Capillary pressure drainage curves may be predicted from NMR T2 distribution when pore size distribution within a sample is homogeneous.

**General information**

**State:** Published

**Organisations:** Department of Environmental Engineering, Center for Energy Resources Engineering, University of Leeds, Chalmers University of Technology

**Authors:** Hossain, Z. (Intern), Grattoni, C. A. (Ekstern), Solymar, M. (Ekstern), Fabricius, I. L. (Intern)

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**Publication date:** 2011

**Main Research Area:** Technical/natural sciences

**Publication information**

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- BFI (2015): BFI-level 1
- Scopus rating (2015): SJR 0.578 SNIP 0.897 CiteScore 1.39
- BFI (2014): BFI-level 1
- Scopus rating (2014): SJR 0.877 SNIP 1.242 CiteScore 1.59
- Web of Science (2014): Indexed yes
- BFI (2013): BFI-level 1
- Scopus rating (2013): SJR 0.866 SNIP 1.285 CiteScore 1.9
- ISI indexed (2013): ISI indexed yes
- BFI (2012): BFI-level 1
- Scopus rating (2012): SJR 1.027 SNIP 1.138 CiteScore 1.56
- ISI indexed (2012): ISI indexed yes
- BFI (2011): BFI-level 1
- Scopus rating (2011): SJR 0.73 SNIP 0.747 CiteScore 1.29
- ISI indexed (2011): ISI indexed yes
- Web of Science (2011): Indexed yes
- BFI (2010): BFI-level 1
- Scopus rating (2010): SJR 1.115 SNIP 1.088
- BFI (2009): BFI-level 1
- Scopus rating (2009): SJR 0.786 SNIP 0.928
- BFI (2008): BFI-level 1
- Scopus rating (2008): SJR 1.023 SNIP 1.28
- Scopus rating (2007): SJR 0.616 SNIP 0.979
- Scopus rating (2006): SJR 0.427 SNIP 0.782
- Scopus rating (2005): SJR 0.614 SNIP 0.872
- Scopus rating (2004): SJR 1.07 SNIP 1.392
- Web of Science (2004): Indexed yes
- Scopus rating (2003): SJR 0.81 SNIP 0.779
- Web of Science (2003): Indexed yes
- Scopus rating (2002): SJR 0.609 SNIP 0.855
- Web of Science (2002): Indexed yes
- Scopus rating (2001): SJR 0.616 SNIP 1.05
- Scopus rating (2000): SJR 0.409 SNIP 0.791
Phase Behavior in EOR Surfactant Flooding

General information
State: Published
Organisations: CERE – Center for Energy Ressources Engineering, Department of Chemical and Biochemical Engineering, Department of Chemistry, Center for Energy Resources Engineering
Authors: Sandersen, S. B. (Intern), von Solms, N. (Intern), Stenby, E. H. (Intern)
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Physical mechanisms of deep bed filtration with application to the problems of petroleum industry

General information
State: Published
Organisations: Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering, Department of Chemistry
Authors: Yuan, H. (Intern), Shapiro, A. (Intern), Stenby, E. H. (Intern)
Publication date: 2011

Publication information
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Publication: Research › Sound/Visual production (digital) – Annual report year: 2011
Pore fluid effect on chalk and clay elasticity

General information
State: Published
Organisations: Section for Geotechnics and Geology, Department of Civil Engineering, Center for Energy Resources Engineering
Authors: Fabricius, I. L. (Intern)
Publication date: 2011

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Title of host publication: Proceedings of Frontiers in diagenesis: Clay & Carbonate facies and their diagenetic pathways in reservoir rocks
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 316122
Publication: Research - peer-review › Conference abstract in proceedings – Annual report year: 2011

Power Consumption in Refrigeration Systems - Modeling for Optimization
Refrigeration systems consume a substantial amount of energy. Taking for instance supermarket refrigeration systems as an example they can account for up to 50−80% of the total energy consumption in the supermarket. Due to the thermal capacity made up by the refrigerated goods in the system there is a possibility for optimizing the power consumption by utilizing load shifting strategies. This paper describes the dynamics and the modeling of a vapor compression refrigeration system needed for sufficiently realistic estimation of the power consumption and its minimization. This leads to a non-convex function with possibly multiple extrema. Such a function can not directly be optimized by standard methods and a qualitative analysis of the system’s constraints is presented. The description of power consumption contains nonlinear terms which are approximated by linear functions in the control variables and the error by doing so is investigated. Finally a minimization procedure for the presented problem is suggested.

General information
State: Published
Organisations: Scientific Computing, Department of Informatics and Mathematical Modeling, Institute for Product Development, Center for Energy Resources Engineering, Danfoss A/S
Authors: Hovgaard, T. G. (Intern), Larsen, L. F. S. (Ekstern), Skovrup, M. J. (Intern), Jørgensen, J. B. (Intern)
Pages: 234-239
Publication date: 2011

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Volume: 2011
Publisher: IEEE
ISBN (Print): 978-1-4244-7460-8
Main Research Area: Technical/natural sciences
Conference: International Symposium on Advanced Control of Industrial Processes, Hangzhou, P.R. China, 01/01/2011
Source: orbit
Source-ID: 270930
Publication: Research - peer-review › Article in proceedings – Annual report year: 2011

Production Optimization of Oil Reservoirs
With an increasing demand for oil and difficulties in nding new major oil elds, research on methods to improve oil recovery from existing elds is more necessary now than ever. The subject of this thesis is to construct ecient numerical methods for simulation and optimization of oil recovery with emphasis on optimal control of water ooding with the use of smartwell technology. We have implemented immiscible ow of water and oil in isothermal reservoirs with isotropic heterogenous permeability elds. We use the method of lines for solution of the partial di erential equation (PDE) system that governs the uid ow. We discretize the the two-phase ow model spatially using the nite volume method (FVM), and we use the two point ux approximation (TPFA) and the single-point upstream (SPU) scheme for computing the uxes. We propose a new formulation of the differential equation system that arise as a consequence of the spatial discretization of the two-phase ow model. Upon discretization in time, the proposed equation system ensures the mass conserving property of the two-phase ow model. For the solution of the spatially discretized two-phase ow model, we develop mass conserving explicit singly diagonally implicit Runge-Kutta (ESDIRK) methods with embedded error estimators for adaptive step size control. We demonstrate that high order ESDIRK methods are more ecient than the low-order methods most commonly used in reservoir simulators. Most commercial reservoir simulation tools use step size control, which is based on heuristics. These can neither deliver solutions with predetermined accuracy or guarantee the convergence in the modied Newton iterations.
We have established predictive step size control based on error estimates, which can be calculated from the embedded ESDIRK methods. We change the step size control in order to minimize the computational cost per simulation. We implement a numerical method for nonlinear model predictive control (NMPC) along with smart-well technology to maximize the net present value (NPV) of an oil reservoir. The optimization is based on quasi-Newton sequential quadratic programming (SQP) with line-search and BFGS approximations of the Hessian, and the adjoint method for efficient computation of the gradients. We demonstrate that the application of NMPC for optimal control of smart-wells has the potential to increase the economic value of an oil reservoir.

**General information**

State: Published
Organisations: Scientific Computing, Department of Informatics and Mathematical Modeling, Center for Energy Resources Engineering
Authors: Völcker, C. (Intern), Jørgensen, J. B. (Intern), Thomsen, P. G. (Intern)
Number of pages: 186
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Original language: English

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Number: 265
Main Research Area: Technical/natural sciences
Electronic versions:
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Source: orbit
Source-ID: 312479
Publication: Research › Ph.D. thesis – Annual report year: 2012

**Quest for consistency, symmetry and simplicity - The legacy of Albert Tarantola**

On 6 December 2009, the distinguished Spanish-French physicist and geoscientist, Albert Tarantola, passed away at the age of 60. Born in Barcelona in 1949, he went to Paris where he lived most of his life, and worked as a professor at Institut de Physique du Globe de Paris. His extensive scientific production and remarkable achievements in inverse problem theory and geophysical data analysis established him as one of the most influential mathematical geoscientists of our time. He became the father of probabilistic inverse theory, a theory that he passionately defended against severe criticism and managed to propagate to a major part of the geophysical community. Another major achievement was his contributions to the theory of seismic waveform inversion — a work that right now is unfolding its potential in large-scale computations. Albert’s contributions were not limited to geoscience. He started his career in astrophysics, and later in his life he wrote several papers and books on physics and probability, including new formulations of fluid dynamics, elasticity theory, global positioning, and scientific inference. Albert possessed a unique combination of exceptional skills and remarkable mental energy. He was a veritable powerhouse with an unusual work ethic, and his passion for science will remain an ideal for all those who worked with him.

**General information**

State: Published
Organisations: Scientific Computing, Department of Informatics and Mathematical Modeling, Center for Energy Resources Engineering
Authors: Mosegaard, K. (Intern)
Pages: W51-W61
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Main Research Area: Technical/natural sciences

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BFI (2018): BFI-level 1
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BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Robust Economic MPC for a Power Management Scenario with Uncertainties

This paper presents a novel incorporation of probabilistic constraints and Second Order Cone Programming (SOCP) with Economic Model Predictive Control (MPC). Hereby the performance of the controller is robustyfied in the presence of both
model and forecast uncertainties. Economic MPC is a receding horizon controller that minimizes an economic objective function and we have previously demonstrated its usage to include a refrigeration system as a controllable power consumer with a portfolio of power generators such that total cost is minimized. The main focus for our work is the power management of the refrigeration system. Whereas our previous study was entirely deterministic, models of e.g. supermarket refrigeration systems are uncertain as is the forecasts of outdoor temperatures and electricity demand. The linear program we have formulated does not cope with uncertainties and thus, such are prone to drive an optimal solution to an infeasible or very expensive solution. The main contribution of this paper is the Finite Impulse Response (FIR) formulation of the system models allowing us to describe and handle model uncertainties in the framework of probabilistic constraints. Our new solution using this setup for robustifying the economic MPC is demonstrated by simulation of a small conceptual example. The scenario is primarily chosen for illustrating the effect of our proposed method in that it can be compared to our previous deterministic simulations.

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Organisations: Scientific Computing, Department of Informatics and Mathematical Modeling, Center for Energy Resources Engineering, Danfoss A/S
Authors: Hovgaard, T. G. (Intern), Larsen, L. F. (Ekstern), Jørgensen, J. B. (Intern)
Pages: 1515-1520
Publication date: 2011

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Source: orbit
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Publication: Research - peer-review › Article in proceedings – Annual report year: 2012

Rock physics model of glauconitic greensand from the North Sea
The objective of this study was to establish a rock physics model of North Sea Paleogene greensand. The Hertz-Mindlin contact model is widely used to calculate elastic velocities of sandstone as well as to calculate the initial sand-pack modulus of the soft-sand, stiff-sand, and intermediate-stiff-sand models. When mixed minerals in rock are quite different, e.g., mixtures of quartz and glauconite in greensand, the Hertz-Mindlin contact model of single type of grain may not be enough to predict elastic velocity. Our approach is first to develop a Hertz-Mindlin contact model for a mixture of quartz and glauconite. Next, we use this Hertz-Mindlin contact model of two types of grains as the initial modulus for a soft-sand model and a stiff-sand model. By using these rock physics models, we examine the relationship between elastic modulus and porosity in laboratory and logging data and link rock-physics properties to greensand diagenesis. Calculated velocity for mixtures of quartz and glauconite from the Hertz-Mindlin contact model for two types of grains are higher than velocity calculated from the Hertz-Mindlin single mineral model using the effective mineral moduli predicted from the Hill's average. Results of rock-physics modeling and thin-section observations indicate that variations in the elastic properties of greensand can be explained by two main diagenetic phases: silica cementation and berthierine cementation. These diagenetic phases dominate the elastic properties of greensand reservoir. Initially, greensand is a mixture of mainly quartz and glauconite; when weakly cemented, it has relatively low elastic modulus and can be modeled by a Hertz-Mindlin contact model of two types of grains. Silica-cemented greensand has a relatively high elastic modulus and can be modeled by an intermediate-stiff-sand or a stiff-sand model. Berthierine cement has different growth patterns in different parts of the greensand, resulting in a soft-sand model and an intermediate-stiff-sand model. © 2012 Society of Exploration Geophysicists.

General information
State: Published
Organisations: Department of Civil Engineering, Section for Geotechnics and Geology, Center for Energy Resources Engineering, Stanford University
Authors: Hossain, Z. (Intern), Mukerji, T. (Ekstern), Dvorkin, J. (Ekstern), Fabricius, I. L. (Intern)
Pages: E199-E209
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Main Research Area: Technical/natural sciences

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BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
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Scopus rating (2016): SJR 1.122 SNIP 1.143 CiteScore 1.53
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.472 SNIP 1.933 CiteScore 2.03
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.413 SNIP 1.434 CiteScore 1.9
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.658 SNIP 2.105 CiteScore 2.25
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Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.693 SNIP 1.837 CiteScore 2.04
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 2.141 SNIP 1.729 CiteScore 2.51
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.755 SNIP 1.716
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.659 SNIP 2.661
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.961 SNIP 1.26
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 0.934 SNIP 1.535
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 0.965 SNIP 2.019
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 0.846 SNIP 1.281
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 0.972 SNIP 2.961
Scopus rating (2003): SJR 0.836 SNIP 2.695
Scopus rating (2002): SJR 0.887 SNIP 1.534
Scopus rating (2001): SJR 0.735 SNIP 1.471
Scopus rating (2000): SJR 0.784 SNIP 1.426
Scopus rating (1999): SJR 0.908 SNIP 1.238
Original language: English
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Screening of amino acid salts solutions for application in CO2 capture from flue gas.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering, Department of Chemistry, CERE – Center for Energy Resources Engineering
Authors: Lerche, B. M. (Intern), Stenby, E. H. (Intern), Thomsen, K. (Intern)
Number of pages: 2
Publication date: 2011
Main Research Area: Technical/natural sciences
CO2 capture, Amino acid salt solution, Flue gas, Solvent properties, CO2 loading capacity, Precipitation, Dynamic flow method
Electronic versions:
- pccc1Abstract00036.pdf
- Presentation_ABDA_2011_BML_sidste.pptx

Bibliographical note
Oral presentation.
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Sonic velocitirs in carbonates. "Shear weakening" is better described as "air stiffening"

General information
State: Published
Organisations: Section for Geotechnics and Geology, Department of Civil Engineering, Center for Energy Resources Engineering, University of Miami
Authors: Fabricius, I. L. (Intern), Eberli, G. P. (Ekstern)
Publication date: 2011
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Main Research Area: Technical/natural sciences
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Source: orbit
Source-ID: 316125
Publication: Research - peer-review › Conference abstract in proceedings – Annual report year: 2011

Strategies for glucose control in people with type 1 diabetes

In this paper we apply a robust feedforward-feedback control strategy to people with type 1 diabetes. The feedforward controller consists of a bolus calculator which compensates the disturbance coming from meals. The feedback controller is based on a linearized description of the model describing the patient. We minimize the risk of hypoglycemia by introducing a time-varying glucose setpoint based on the announced meal size and the physiological model of the patient. The simulation results are based on a virtual patient simulated by the Hovorka model. They include the cases where the insulin sensitivity changes, and mismatches in meal estimation. They demonstrate that the designed controller is able to achieve offset-free control when the insulin sensitivity change, and that having a time-varying reference signal enables more robust control of blood glucose in the cases where the meal size is known, but also when the ingested meal does not match the announced one.

General information
State: Published
Organisations: Center for Energy Resources Engineering, Department of Informatics and Mathematical Modeling, Scientific Computing, Mathematical Statistics
Sulfur Release from Cement Raw Materials during Solid Fuel Combustion

During combustion of solid fuels in the material inlet end of cement rotary kilns, local reducing conditions can occur and cause decomposition of sulfates from cement raw materials. Decomposition of sulfates is problematic because it increases the gas-phase SO2 concentration, which may cause deposit formation in the kiln system. SO2 release from cement raw materials during combustion of solid fuels has been studied experimentally in a high temperature rotary drum. The fuels were tire rubber, pine wood, petcoke, sewage sludge, and polypropylene. The SO2 release from the raw materials was observed to increase when (a) the inlet oxygen concentration decreased, (b) the temperature increased, and (c) when the total surface area of the fuel particles increased. The type of fuel also had a significant effect on the SO2 release. The sequence of SO2 release for fuel particles in the size interval 1–2 mm was found to be tire rubber granulate > sewage sludge > pine wood sawdust > petcoke > polypropylene flakes. The SO2 release was generally observed to increase when formation of local reducing conditions near the raw material bed increased, as indicated by elevated levels of CO during the fuel devolatilization.
Systematic identification and robust control design for uncertain time delay processes

A systematic procedure is proposed to handle the standard process control problem. The considered standard problem involves infrequent step disturbances to processes with large delays and measurement noise. The process is modeled as an ARX model and extended with a suitable noise model in order to reject unmeasured step disturbances and unavoidable model errors. This controller is illustrated to perform well for both set point tracking and a disturbance rejection for a SISO process example of a furnace which has a time delay which is significantly longer than the dominating time constant.

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, Mathematical Statistics, Department of Informatics and Mathematical Modeling, Scientific Computing, Center for Energy Resources Engineering
Authors: Huusom, J. K. (Intern), Poulsen, N. K. (Intern), Jørgensen, S. B. (Intern), Jørgensen, J. B. (Intern)
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Main Research Area: Technical/natural sciences
Systematic identification and robust control design for uncertain time delay processes

Advanced control strategies such as Model Predictive Control have gained wide spread interest in many areas in the chemical industries, due to fast algorithms, a well established theory and growing number of successful industrial implementations. The main feature is that the optimal control signal is determined as a constrained optimization which utilizes future predictions of the plant behaviour. Hence the controller has a plant model embedded for state estimation. The achieved closed loop performance is therefore dependent on the quality of the future predictions. The performance of the state estimator is on the other hand dependent on the accuracy of the process and the noise model. Systems with long delays in the dynamic response between the actuators and the controlled variables are notoriously difficult to control or tune. A model predictive control implementation based on a model with the correct delay will provide good set-point tracking performance as long as the prediction horizon of the controller is longer than the delay. Hence a predictive controller would perform better in rejecting known disturbances and changes between operation modes than a PI controller with time-delay compensation as e.g. a Smith predictor. A common problem for all controllers, operating on a system with a delay longer than the dominating time constant, is that a stable system may reject small disturbances before the controller have an opportunity to act. If the controller is tuned to react on these minor disturbances the change in the actuator would lead to an increase in the variance of the system output. It is therefore desired if the controller does not react on minor disturbances or measurement noise. It is on the other hand important that the controller is not detuned such that significant or sustained disturbances cannot be effectively rejected. We proposed a model predictive control implementation with a dead-band on the penalty of the tracking error as a mean to achieve good closed loop performance on time delay system. We have in simulation tested our controller on a SISO system of an industrial furnace and a MIMO system on a cement grinding circuit.

Uncertainty and Sensitivity Analysis of Filtration Models for Non-Fickian transport and Hyperexponential deposition

Uncertainty and sensitivity analyses are carried out to investigate the predictive accuracy of the filtration models for describing non-Fickian transport and hyperexponential deposition. Five different modeling approaches, involving the elliptic equation with different types of distributed filtration coefficients and the CTRW equation expressed in Laplace space, are selected to simulate eight experiments. These experiments involve both porous media and colloid-medium interactions of different heterogeneity degrees. The uncertainty of elliptic equation predictions with distributed filtration coefficients is larger than that with a single filtration coefficient. The uncertainties of model predictions from the elliptic equation and CTRW equation in Laplace space are minimal for solute transport. Higher uncertainties of parameter estimation and model outputs are observed in the cases with the porous media and the colloid-medium interactions of higher heterogeneity. The parameters for the distribution of filtration coefficients could not be uniquely identified due to strong correlations. In the cases of heterogeneous colloid-medium interactions where hyper-exponential deposition is observed, the distribution of filtration coefficients could not be accurately determined by the effluent concentration profile alone. Measurements of deposition are necessary. The effluent concentrations around the breakthrough and around the end of colloid injection are more sensitive to dispersion coefficients than filtration coefficients, while deposition is more sensitive to filtration coefficients. More experimental measurements at these moments are suggested to determine dispersion coefficients more accurately. More measurements of the steady-state effluent concentration or deposition are suggested to determine filtration coefficients more accurately.
1D Simulations for Microbial Enhanced Oil Recovery with Metabolite Partitioning

We have developed a mathematical model describing the process of microbial enhanced oil recovery (MEOR). The one-dimensional isothermal model comprises displacement of oil by water containing bacteria and substrate for their feeding. The bacterial products are both bacteria and metabolites. In the context of MEOR modeling, a novel approach is...
partitioning of metabolites between the oil and the water phases. The partitioning is determined by a distribution coefficient. The transfer part of the metabolite to oil phase is equivalent to its "disappearance", so that the total effect from of metabolite in the water phase is reduced. The metabolite produced is surfactant reducing oil–water interfacial tension, which results in oil mobilization. The reduction of interfacial tension is implemented through relative permeability curve modifications primarily by lowering residual oil saturation. The characteristics for the water phase saturation profiles and the oil recovery curves are elucidated. However, the effect from the surfactant is not necessarily restricted to influence only interfacial tension, but it can also be an approach for changing, e.g., wettability. The distribution coefficient determines the time lag, until residual oil mobilization is initialized. It has also been found that the final recovery depends on the distance from the inlet before the surfactant effect takes place. The surfactant effect position is sensitive to changes in maximum growth rate, and injection concentrations of bacteria and substrate, thus determining the final recovery. Different methods for incorporating surfactant-induced reduction of interfacial tension into models are investigated. We have suggested one method, where several parameters can be estimated in order to obtain a better fit with experimental data. For all the methods, the incremental recovery is very similar, only coming from small differences in water phase saturation profiles. Overall, a significant incremental oil recovery can be achieved, when the sensitive parameters in the context of MEOR are carefully dealt with.
Absorber Model for CO2 Capture by Monoethanolamine

The rate-based steady-state model proposed by Gabrielsen et al. (Gabrielsen, J.; Michelsen, M. L.; Kontogeorgis, G. M.; Stenby, E. H. AIChE J. 2006, 52, 10, 3443-3451) for the design of the CO2-2-amino-2-methylpropanol absorbers is adopted and improved for the design of the CO2-monoethanolamine absorber. The influence of the application of different mass transfer correlations on the model's performance is investigated. Analytical expressions for the calculation of the enhancement factor for the second order as well as the pseudo-first-order reaction regime are integrated in the model, and their impact on the model's prediction is compared. The model has been successfully applied to CO2 absorber packed columns and validated against pilot plant data with good agreement.

General information
State: Published
Organisations: CERE – Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Faramarzi, L. (Intern), Kontogeorgis, G. (Intern), Michelsen, M. L. (Intern), Thomsen, K. (Intern), Stenby, E. H. (Intern)
Pages: 3751-3759
Publication date: 2010
Main Research Area: Technical/natural sciences

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BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.1 SJR 0.945 SNIP 1.139
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.949 SNIP 1.146 CiteScore 2.87
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2

Absorber Model for CO2 Capture by Monoethanolamine

The rate-based steady-state model proposed by Gabrielsen et al. (Gabrielsen, J.; Michelsen, M. L.; Kontogeorgis, G. M.; Stenby, E. H. AIChE J. 2006, 52, 10, 3443-3451) for the design of the CO2-2-amino-2-methylpropanol absorbers is adopted and improved for the design of the CO2-monoethanolamine absorber. The influence of the application of different mass transfer correlations on the model's performance is investigated. Analytical expressions for the calculation of the enhancement factor for the second order as well as the pseudo-first-order reaction regime are integrated in the model, and their impact on the model's prediction is compared. The model has been successfully applied to CO2 absorber packed columns and validated against pilot plant data with good agreement.
A Dantzig-Wolfe MPC Algorithm for Power Plant Portfolio Control

General information
State: Submitted
Organisations: Scientific Computing, Department of Informatics and Mathematical Modeling, Center for Energy Resources Engineering
Authors: Edlund, K. (Ekstern), Jørgensen, J. B. (Intern)
Publication date: 2010
Adaptive Step Size Control in Implicit Runge-Kutta Methods for Reservoir Simulation
Application of Soft Constrained MPC to a Cement Mill Circuit

General information
ARX-based Model Predictive Control of Systems with Time Delays

General information
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Organisations: Department of Chemical and Biochemical Engineering, Mathematical Statistics, Department of Informatics and Mathematical Modeling, Computer Aided Process Engineering Center, Center for Energy Resources Engineering
Authors: Huusom, J. K. (Intern), Poulsen, N. K. (Intern), Jørgensen, S. B. (Intern), Jørgensen, J. B. (Intern)
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Publication date: 2010

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Source-ID: 252801
Publication: Research - peer-review › Article in proceedings – Annual report year: 2010

ARX-Model based Model Predictive Control with Offset-Free Tracking

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Authors: Huusom, J. K. (Intern), Poulsen, N. K. (Intern), Jørgensen, S. B. (Intern), Jørgensen, J. B. (Intern)
Publication date: 2010

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Conference: 20th European Symposium on Computer Aided Process Engineering, Ischia, Italy, 06/06/2010 - 06/06/2010
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Source-ID: 252801
Publication: Research - peer-review › Article in proceedings – Annual report year: 2010
ARX MPC for people with type 1 diabetes
Type 1 diabetes is a chronic disease characterized by a lack of production of pancreatic insulin, consequently leading to high blood glucose concentrations (hyperglycemia). Hyperglycemia has negative health effects in the long term such as eye, nerve, and kidney disease. Exogenous insulin must be injected to keep the blood glucose in the normoglycemic range (approximately 60 – 140 mg/dL, or 3.3 – 8 mmol/L). However, the dosing of exogenous insulin must be done carefully, because low blood glucose concentrations (hypoglycemia) can have immediate and severe consequences like insulin shock, coma, or even death. Currently, insulin administration is performed by the subject with type 1 diabetes based on infrequent glucose measurements (in the form of finger-sticks), often resulting in an unsatisfactory blood glucose control. An artificial pancreas is a medical device that injects exogenous insulin automatically in order to regulate the glucose concentration. Blood glucose measurements are obtained from a continuous glucose monitor (CGM). Insulin is administrated either continuously through an insulin pump, or at discrete times using an insulin pen. A control algorithm uses previous glucose measurements and insulin injection information to compute the optimal insulin administration for the current conditions. We use model predictive control (MPC) to compute the optimal insulin administration for 20 virtual type 1 diabetes subjects. The system (i.e., subject) has one manipulated input (insulin infusion rate), one disturbance input (carbohydrate meals), and one measured output (blood glucose concentration). The subject is represented by a system of nonlinear differential equations describing the dynamic effects of insulin and meals on blood glucose. Twenty parameter sets are used in the study, each representing a different virtual subject. The model used in the MPC is a low order autoregressive exogenous-input (ARX) model. Due to both the linearity and relative parsimony of the ARX model, there is a significant amount of subject/model mismatch in the model predictions, reflecting real-world conditions. In general, a simple ARX MPC cannot reject a step disturbance without a resulting offset; thus, the state vector is reformulated using an extended ΔARX description (E-ΔARX). The reference signal is time-varying, and is based on the optimal open-loop glucose profile. Insulin-on-board constraints are implemented to avoid overdosing insulin. State estimation is based on a Kalman filter using the noise model to simulate a realistic CGM. We present the MPC results for simulations of the 20 virtual subjects with type 1 diabetes. In particular, we investigate the effects of the prediction horizon length on the control quality of blood glucose and the robustness of the solution.

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Organisations: Scientific Computing, Department of Informatics and Mathematical Modeling, Mathematical Statistics, Center for Energy Resources Engineering
Publication date: 2010
Main Research Area: Technical/natural sciences
Type 1 diabetes, ARX model, Model predictive control, Kalman filtering
Electronic versions: Abstract2.pdf
Source: orbit
Source-ID: 262936
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2010

A Stochastic Theory for Deep Bed Filtration Accounting for Dispersion and Size Distributions
We develop a stochastic theory for filtration of suspensions in porous media. The theory takes into account particle and por size distributions, as well as the random character of the particle motion, which is described in the framework of the theory of continuous-time random walks (CTRW). In the limit of the infinitely many small walk steps we derive a system of governing equations for the evolution of the particle and pore size distributions. We consider the case of concentrated suspensions, where plugging the pores by particles may change porosity and other parameters of the porous medium. A procedure for averaging of the derived system of equations is developed for polydisperse suspensions with several distinctive particle sizes. A numerical method for solution of the flow equations is proposed. Sample calculations are applied to compare the roles of the particle size distribution and of the particle flight dispersion on the deposition profiles. It is demonstrated that the temporal flight dispersion is the most likely mechanism forming the experimentally observed hyperexponential character of the deposition profiles.

General information
State: Published
Organisations: CERE – Center for Energy Ressources Engineering, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Shapiro, A. (Intern), Bedrikovetsky, P. G. (Ekstern)
Injection of water into chalk hydrocarbon reservoirs has led to mechanical yield and failure. Laboratory experiments on chalk samples correspondingly show that the mechanical properties of porous chalk depend on pore fluid and temperature. Water has a significant softening effect on elastic properties of chalk as calculated from wave data, and the softening increases with increasing critical frequency as defined by Biot. The critical frequency is the highest frequency where wave propagation is controlled by solid-fluid friction. The Biot critical frequency is thus a measure of this friction and we propose that the fluid effect on mechanical properties of highly porous chalk may be the result of liquid-solid friction. Applying a different strain or stress rate is influencing the rock strength and needs to be included. The resulting function is shown to relate to the material dependent and rate independent b-factor used when describing the time dependent mechanical properties of soft rock or soils. As a consequence it is then possible to further characterize the material constant from the porosity and permeability of the rock as well as from pore fluid density and viscosity which is highly influenced by temperature.

**Biot Critical Frequency Applied as Common Friction Factor for Pore Collapse and Failure of Chalk with Different Pore Fluids and Temperatures**

**General information**
- State: Published
- Organisations: Section for Geotechnics and Geology, Department of Civil Engineering, Department of Environmental Engineering, Center for Energy Resources Engineering
- Authors: Andreassen, K. A. (Intern), Fabricius, I. L. (Intern)
- Pages: 1-10
- Publication date: 2010

**Host publication information**
- Title of host publication: 44th US Rock Mechanics Symposium : 5th U.S. -Canada Rock Mechanics Symposium
- Volume: Proceedings-DVD
- Main Research Area: Technical/natural sciences
- Conference: 44th US Rock Mechanics Symposium and 5th U.S. -Canada Rock Mechanics Symposium, Salt Lake City, USA, 01/01/2010
- Source: orbit
- Source-ID: 270967
- Publication: Research - peer-review › Article in proceedings – Annual report year: 2010

Biot Critical Frequency Applied to Description of Failure and Yield of Highly Porous Chalk with Different Pore Fluids

Injection of water into chalk hydrocarbon reservoirs has led to mechanical yield and failure. Laboratory experiments on chalk samples correspondingly show that the mechanical properties of porous chalk depend on pore fluid and temperature. In case of water-saturated samples, the concentration and nature of dissolved salts have an effect. Water has a significant softening effect on elastic properties of chalk as calculated from wave data, and the softening increases with increasing critical frequency as defined by Biot. The critical frequency is the highest frequency where wave propagation is controlled by solid-fluid friction. The reference frequency is thus a measure of this friction, and we propose...
that the fluid effect on mechanical properties of chalk may be the result of liquid-solid friction. We reviewed 622 published experiments on mechanical properties of porous chalk. The data include chalk samples that were tested at temperatures from 20 °C to 130 °C with the following pore fluids: fresh water, synthetic seawater, glycol, and oil of varying viscosity. The critical frequency is calculated for each experiment. For each specimen, we calculate the thickness to the slipping plane outside the Stern layer on the pore surface. For electrolytes, the thickness of this layer is calculated based on Debye-Hückel theory. The layer reduces the porosity available for fluid flow. We find that the Biot critical frequency based on pore scale data can be used to explain effects on the macro scale. We find that the effective yield stress and also the effective stress of failure in tension as well as in compression are log-linearly related to log reference frequency. This opens the possibility to predict yield and failure under reservoir conditions from mechanical tests made under laboratory conditions. It also opens the possibility of predicting the effects of water flooding on chalk stability.

General information
State: E-pub ahead of print
Organisations: Department of Civil Engineering, Department of Environmental Engineering, Center for Energy Resources Engineering
Authors: Andreassen, K. A. (Intern), Fabricius, I. L. (Intern)
Pages: E205-E213
Publication date: 2010
Main Research Area: Technical/natural sciences

Publication information
Journal: Geophysics
Volume: 75
Issue number: 6
ISSN (Print): 0016-8033
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BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 1.122 SNIP 1.143 CiteScore 1.53
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.472 SNIP 1.933 CiteScore 2.03
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.413 SNIP 1.434 CiteScore 1.9
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.658 SNIP 2.105 CiteScore 2.25
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.693 SNIP 1.837 CiteScore 2.04
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 2.141 SNIP 1.729 CiteScore 2.51
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.755 SNIP 1.716
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.659 SNIP 2.661
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Biot’s coefficient as an indicator of strength and porosity reduction: Calcareous sediments from Kerguelen Plateau

Chalk develops as a result of diagenesis of pelagic calcareous ooze. In a newly deposited ooze sediment, porosity ranges from 60% to 80% but porosity reduces with burial. We studied how different porosity reduction mechanisms change the strength of these deep sea carbonate-rich sediments and effect Biot’s coefficient, $\beta$. In calcareous ooze, $\beta$ is one. Mechanical compaction reduces porosity, but only leads to a minor decrease in $\beta$. Recrystallization renders particles smoother, but does not lead to reduction in $\beta$ unless it gives rise to pore stiffening cementation. Pore stiffening cementation causes $\beta$ to fall, even when porosity remains constant. Biot's coefficient correlates with strength-indicating properties: compressional and shear modulus, oedometer modulus, yield strength, strain from direct loading and creep strain. Our data indicate that $\beta$ may be used for predicting the diagenetic process involved in porosity reduction and strengthening of chalk during burial diagenesis.

General information
State: Published
Organisations: Department of Environmental Engineering, Section for Geotechnics and Geology, Department of Civil Engineering, Center for Energy Resources Engineering
Authors: Alam, M. M. (Intern), Borre, M. K. (Intern), Fabricius, I. L. (Intern), Hedegaard, K. (Intern), Røgen, B. (Intern), Hossain, Z. (Intern), Krogsbøll, A. S. (Intern)
Pages: 282-297
Publication date: 2010
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Petroleum Science and Engineering
Volume: 70
Issue number: 3-4
ISSN (Print): 0920-4105
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.56 SJR 0.764 SNIP 1.631
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.801 SNIP 1.652 CiteScore 2.38
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Creep of Highly Porous Chalk and Biot Critical Frequency

General information
State: Published
Organisations: Section for Geotechnics and Geology, Department of Civil Engineering, Department of Environmental Engineering, Center for Energy Resources Engineering
Authors: Andreassen, K. A. (Intern), Fabricius, I. L. (Intern), Foged, N. N. (Intern)
Pages: 1-2
Publication date: 2010

Host publication information
Title of host publication: A new spring for geoscience : 72nd EAGE conference and exhibition, Barcelona 14-17 June 2010 : Conference proceedings & exhibitors' catalogue. CD-ROM / Editor - DB Houten, NL : EAGE, 2010
ISBN (Print): 978-90-73781-86-3
Main Research Area: Technical/natural sciences
Conference: 72nd EAGE Conference & Exhibition incorporating SPE EUROPEC 2010, Barcelona, Spain, 14/06/2010 - 14/06/2010
Elastic moduli of dry and water-saturated carbonates - Effect of depositional texture, porosity, and permeability

General information
State: Published
Organisations: Department of Environmental Engineering, Center for Energy Resources Engineering
Authors: Fabricius, I. L. (Intern), Bächle, G. (Ekstern), Eberli, G. (Ekstern)
Pages: N65-N78
Publication date: 2010
Main Research Area: Technical/natural sciences

Publication information
Journal: Geophysics
Volume: 75
Issue number: 3
ISSN (Print): 0016-8033
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 1.122 SNIP 1.143 CiteScore 1.53
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.472 SNIP 1.933 CiteScore 2.03
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.413 SNIP 1.434 CiteScore 1.9
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.658 SNIP 2.105 CiteScore 2.25
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.693 SNIP 1.837 CiteScore 2.04
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 2.141 SNIP 1.729 CiteScore 2.51
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.755 SNIP 1.716
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.659 SNIP 2.661
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.961 SNIP 1.26
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 0.934 SNIP 1.535
Explicit Singly Diagonally Implicit Runge-Kutta Methods and Adaptive Stepsize Control for Reservoir Simulation

The implicit Euler method, normally referred to as the fully implicit (FIM) method, and the implicit pressure explicit saturation (IMPES) method are the traditional choices for temporal discretization in reservoir simulation. The FIM method offers unconditionally stability in the sense of discrete approximations, while the IMPES scheme benefits from the explicit treatment of the saturation. However, in terms of controlling the integration error, the low order of the FIM method leads to small integration steps, while the explicit treatment of the saturation may restrict the stepsizes for the IMPES scheme. Current reservoir simulators apply timestepping algorithms that are based on safeguarded heuristics, and can neither guarantee convergence in the underlying equation solver, nor provide estimates of the relations between convergence, integration error and stepsizes. We establish predictive stepsize control applied to high order methods for temporal discretization in reservoir simulation. The family of Runge-Kutta methods is presented and in particular the explicit singly diagonally implicit Runge-Kutta (ESDIRK) method with an embedded error estimate is described. A predictive stepsize adjustment rule based on error estimates and convergence control of the integrated iterative solver is presented. We try to improve the predictive stepsize control through an extended communication between the convergence rate, the error control and the stepsize. Keywords: Reservoir simulation, implicit Runge-Kutta methods, ESDIRK, Newton-Raphson, convergence control, error control, stepsize selection.

Geostatistical inference using crosshole ground-penetrating radar

High-resolution tomographic images obtained from crosshole geophysical measurements have the potential to provide valuable information about the geostatistical properties of unsaturated-zone hydrologic-state variables such as moisture content. Under drained or quasi-steady-state conditions, the moisture content will reflect the variation of the physical properties of the subsurface, which determine the flow patterns in the unsaturated zone. Deterministic least-squares inversion of crosshole ground-penetrating-radar GPR traveltimes result in smooth, minimum-variance estimates of the subsurface radar wave velocity structure, which may diminish the utility of these images for geostatistical inference. We have used a linearized stochastic inversion technique to infer the geostatistical properties of the subsurface radar wave velocity distribution using crosshole GPR traveltimes directly. Expanding on a previous study, we have determined that it is possible to obtain estimates of global variance and mean velocity values of the subsurface as well as the correlation lengths describing the subsurface velocity structures. Accurate estimation of the global variance is crucial if stochastic realizations of the subsurface are used to evaluate the uncertainty of the inversion estimate. We have explored the full potential of the geostatistical inference method using several synthetic models of varying correlation structures and have
tested the influence of different assumptions concerning the choice of covariance function and data noise level. In addition, we have tested the methodology on traveltime data collected at a field site in Denmark. There, inferred correlation structures indicate that structural differences exist between two areas located approximately 10 m apart, an observation confirmed by a GPR reflection profile. Furthermore, the inferred values of the subsurface global variance and the mean velocity have been corroborated with moisture content measurements, obtained gravimetrically from samples collected at the field site.

General information
State: Published
Organisations: Department of Informatics and Mathematical Modeling, Scientific Computing, Center for Energy Resources Engineering, Lancaster University, University of Copenhagen
Authors: Looms, M. C. (Ekstern), Hansen, T. M. (Intern), Cordua, K. S. (Intern), Nielsen, L. (Ekstern), Jensen, K. H. (Ekstern), Binley, A. (Ekstern)
Pages: J29-J41
Publication date: 2010
Main Research Area: Technical/natural sciences

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Journal: Geophysics
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BFI (2018): BFI-level 1
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Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 1.122 SNIP 1.143 CiteScore 1.53
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.472 SNIP 1.933 CiteScore 2.03
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.413 SNIP 1.434 CiteScore 1.9
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.658 SNIP 2.105 CiteScore 2.25
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.693 SNIP 1.837 CiteScore 2.04
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 2.141 SNIP 1.729 CiteScore 2.51
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.755 SNIP 1.716
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.659 SNIP 2.661
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.961 SNIP 1.26
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 0.934 SNIP 1.535
Implications and Limitations of Ideal Insulin Administration for People with Type 1 Diabetes

General information
State: Published
Organisations: Center for Energy Resources Engineering, Department of Informatics and Mathematical Modeling, Scientific Computing, Mathematical Statistics
Publication date: 2010

Host publication information
Title of host publication: UKACC International Conference on CONTROL 2010 proceedings
Main Research Area: Technical/natural sciences
Conference: UKACC International Conference on CONTROL, Coventry, United Kingdom, 01/01/2010
Electronic versions:
UKACC2010.pdf
Source: orbit
Source-ID: 266921
Publication: Research - peer-review › Article in proceedings – Annual report year: 2010

Inhibition of Methane Hydrate Formation by Ice-Structuring Proteins

In the oil and gas industry there is ample motivation for moving toward greener kinetic inhibitors of gas hydrates as many of those used today suffer from poor biodegradability. In this work, we have investigated experimentally whether ice-structuring proteins (ISPs) found in fish and insect, assumed biodegradable, are capable of inhibiting the growth of methane hydrate (a structure I hydrate). The ISPs investigated were type III HPLC12 (originally identified in ocean pout) and ISP type III found in meal worm (Tenebrio molitor). These were compared to polyvinylpyrrolidone (PVP) a well-known kinetic hydrate inhibitor. The results revealed that adding ISP in sufficient amounts caused the appearance of an initial nonlinear growth period. At a certain point during the growth process the growth pattern changed to linear which is identical to the growth observed for methane hydrate in the absence of inhibitors. The profile of the nonlinear growth was concentration-dependent but also dependent on the stirring rate. ISP type III HPLC12 decreased the growth rate of methane hydrate during the linear growth period by 17−75% at concentrations of 0.01−0.1 wt % (0.014−0.14 mM) while ISP from Tenebrio molitor and PVP decreased the growth rate by 30% and 39% at concentrations of 0.004 wt % (0.005 mM) and 0.1 wt % (0.1 mM), respectively. Considering the low concentration of Tenebrio molitor ISP used, these results indicate that ISP from Tenebrio molitor is the most effective hydrate inhibitor among those investigated. Thermal hysteresis ice formation experiments revealed that ISP from Tenebrio molitor causes higher thermal hysteresis for ice formation compared to type III ISP identified in ocean pout while PVP did not cause thermal hysteresis. This indicates that there might be a direct relationship between ISP performance for ice and hydrate inhibition, and that thermal hysteresis experiments can be used to screen ISPs as kinetic inhibitors.

General information
State: Published
Organisations: CERE – Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Kriging in High Dimensional Attribute Space using Principal Component Analysis

General information
State: Published
Organisations: Scientific Computing, Department of Informatics and Mathematical Modeling, Center for Energy Resources Engineering
Authors: Lange, K. (Intern), Fernández Martínez, J. L. (Ekstern), Frydendall, J. (Intern), Mosegaard, K. (Intern)
Publication date: 2010

Host publication information
Title of host publication: IAMG Extended Abstracts
Main Research Area: Technical/natural sciences
Conference: 14th Annual Conference of the International Association for Mathematical Geosciences, Budapest, Hungary, 29/08/2010 - 29/08/2010
Source: orbit
Source-ID: 270885
Publication: Research › Article in proceedings – Annual report year: 2010

Kriging Interpolation in Seismic Attribute Space Applied to the South Arne Field, North Sea
Seismic attributes can be used to guide interpolation in-between and extrapolation away from well log locations using for example linear regression, neural networks, and kriging. Kriging-based estimation methods (and most other types of interpolation/extrapolation techniques) are intimately linked to distances in physical space. If two observations are located close to one another, the implicit assumption is that they are highly correlated. This may, however, not be a correct assumption as the two locations can be situated in very different geological settings. An alternative approach to the traditional kriging implementation is suggested that frees the interpolation from the restriction of the physical space. The method is a fundamentally different application of the original kriging formulation where a model of spatial variability is replaced by a model of variability in an attribute space. To the extent that subsurface geology can be described by a set of seismic attributes, we present an automated multivariate kriging-based interpolation method that is guided by geological similarity rather than by the conventional distance measure in XYZ space. Through a case study, kriging in attribute space is used to estimate 2D porosity maps from a number of well logs and seismic attributes in the Danish North Sea. Cokriging provides uncertainty estimates that are dependent on the primary data locations in space, whereas kriging in attribute space provides uncertainty estimates that reflect subsurface geological variability. The North Sea case study demonstrates that kriging in attribute space performs better than linear regression and cokriging.

General information
State: Published
Organisations: Scientific Computing, Department of Informatics and Mathematical Modeling, Center for Energy Resources Engineering, Hess Denmark
Authors: Hansen, T. M. (Intern), Mosegaard, K. (Intern), Schiøtt, C. (Ekstern)
Pages: 31-41
Publication date: 2010
Main Research Area: Technical/natural sciences

Publication information
Journal: Geophysics
Volume: 75
Issue number: 6
ISSN (Print): 0016-8033
Ratings:
Meal Estimation in Nonlinear Model Predictive Control for Type 1 Diabetes

General information
State: Published
Organisations: Center for Energy Resources Engineering, Department of Informatics and Mathematical Modeling, Scientific Computing, Mathematical Statistics
Pages: 1052-1057
Publication date: 2010

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Title of host publication: 8th IFAC Symposium on Nonlinear Control Systems
Main Research Area: Technical/natural sciences
Conference: 8th IFAC Symposium on Nonlinear Control Systems, 01/01/2010
Source: orbit
Source-ID: 259673
Publication: Research - peer-review › Article in proceedings – Annual report year: 2010

Modeling and Simulation of Single Cell Protein Production

General information
State: Published
Organisations: Scientific Computing, Department of Informatics and Mathematical Modeling, Center for BioProcess Engineering, Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Center for Energy Resources Engineering
Authors: Olsen, D. F. (Ekstern), Jørgensen, J. B. (Intern), Villadsen, J. (Intern), Jørgensen, S. B. (Intern)
Pages: 502-507
Publication date: 2010

Host publication information
Title of host publication: 11th Computer Applications in Biotechnology
Main Research Area: Technical/natural sciences
Conference: 11th Computer Applications in Biotechnology, Leuven, Belgium, 07/07/2010 - 07/07/2010
Source: orbit
Source-ID: 259667
Publication: Research - peer-review › Article in proceedings – Annual report year: 2010

Modeling and Simulation of Single Cell Protein Production

General information
State: Published
Organisations: Scientific Computing, Department of Informatics and Mathematical Modeling, Center for BioProcess Engineering, Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Center for Energy Resources Engineering
Authors: Olsen, D. F. (Ekstern), Jørgensen, J. B. (Intern), Villadsen, J. (Intern), Jørgensen, S. B. (Intern)
Publication date: 2010

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 266290
Publication: Research › Sound/Visual production (digital) – Annual report year: 2010

Modeling Reservoir Formation Damage due to Water Injection for Oil Recovery

The elliptic equation for non-Fickian transport of suspension in porous media is applied to simulate the reservoir formation damage due to water injection for oil recovery. The deposition release (erosion of reservoir formation) and the suspension deposition (pore plugging) are both taken into account. 1-D numerical simulations are carried out to reveal the erosion of reservoir formation due to water injection. 2-D numerical simulations are carried out to obtain the suspension and deposition profiles around the injection wells. These preliminary results indicate the non-Fickian behaviors of suspended reservoir fines and the corresponding formation damage due to erosion and relocation of reservoir fines.
Model predictive control for plant-wide control of a reactor-separator-recycle system

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Scientific Computing, Department of Informatics and Mathematical Modeling, Computer Aided Process Engineering Center, Center for Energy Resources Engineering
Authors: Bialas, D. J. (Ekstern), Huusom, J. K. (Intern), Jørgensen, J. B. (Intern), Sin, G. (Intern)
Publication date: 2010

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 265529
Publication: Research › Sound/Visual production (digital) – Annual report year: 2010

Model predictive control for reactor-separator-recycle system

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Scientific Computing, Department of Informatics and Mathematical Modeling, Computer Aided Process Engineering Center, Center for Energy Resources Engineering
Authors: Bialas, D. J. (Ekstern), Huusom, J. K. (Intern), Jørgensen, J. B. (Intern), Sin, G. (Intern)
Number of pages: 145
Publication date: 2010

Host publication information
Title of host publication: Proceedings of Dansk Kemiingeniørkonference 2010
Main Research Area: Technical/natural sciences
Conference: 3. Dansk KemiingeniørKonference, Kgs. Lyngby, Denmark, 16/06/2010 - 16/06/2010
Source: orbit
Source-ID: 265907
Publication: Research › Article in proceedings – Annual report year: 2010

Model predictive control for reactor-separator-recycle system

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Scientific Computing, Department of Informatics and Mathematical Modeling, Computer Aided Process Engineering Center, Center for Energy Resources Engineering
Authors: Bialas, D. J. (Ekstern), Huusom, J. K. (Intern), Jørgensen, J. B. (Intern), Sin, G. (Intern)
Publication date: 2010

Main Research Area: Technical/natural sciences
Source: orbit
Model Predictive Control for Smart Energy Systems

General information
State: Published
Organisations: Center for Energy Resources Engineering, Department of Informatics and Mathematical Modeling, Scientific Computing
Authors: Jørgensen, J. B. (Intern), Edlund, K. (Ekstern), Hovgaard, T. G. (Intern), Sokoler, L. E. (Ekstern)
Publication date: 2010

Monte Carlo full waveform inversion of tomographic crosshole data using complex geostatistical a priori information

General information
State: Published
Organisations: Scientific Computing, Department of Informatics and Mathematical Modeling, Center for Energy Resources Engineering
Authors: Cordua, K. S. (Intern), Hansen, T. M. (Intern), Mosegaard, K. (Intern)
Publication date: 2010

Nonlinear AVO inversion using geostatistical a priori information

General information
State: Published
Organisations: Scientific Computing, Department of Informatics and Mathematical Modeling, Center for Energy Resources Engineering
Authors: Cordua, K. S. (Intern), Hansen, T. M. (Intern), Mosegaard, K. (Intern)
Publication date: 2010

Nonlinear Model Predictive Control for an Artificial Beta-Cell

General information
State: E-pub ahead of print
Organisations: Scientific Computing, Department of Informatics and Mathematical Modeling, Mathematical Statistics, Center for Energy Resources Engineering
Pages: 299-308
Publication date: 2010
Optimal Insulin Administration for People with Type 1 Diabetes

General information
State: Published
Organisations: Scientific Computing, Department of Informatics and Mathematical Modeling, Mathematical Statistics, Center for Energy Resources Engineering
Publication date: 2010

Optimal Operating Points for SCP Production in the U-Loop Reactor

General information
State: Published
Organisations: Scientific Computing, Department of Informatics and Mathematical Modeling, Center for BioProcess Engineering, Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Center for Energy Resources Engineering
Authors: Olsen, D. F. (Ekstern), Jørgensen, J. B. (Intern), Villadsen, J. (Intern), Jørgensen, S. B. (Intern)
Publication date: 2010
ParPor: Particles in Pores. Stochastic Modeling of Polydisperse Transport

Liquid flow containing particles in the different types of porous media appear in a large variety of practically important industrial and natural processes. The project aims at developing a stochastic model for the deep bed filtration process in which the polydisperse suspension flow in the polydisperse porous media. Instead of the traditional parabolic Advection-Dispersion Equation (ADE) the novel elliptic PDE based on the Continuous Time Random Walk is adopted for the particle size kinetics. The pore kinetics is either described by the stochastic size exclusion mechanism or the incomplete pore plugging model. In the current phase of the project the computation is only performed for the polydisperse suspension flow in monodisperse porous media. The slower transport speed of the peak and larger tail indicates that the elliptic model is more adaptable for anomalous diffusion. Porosity decline of the porous media and convection acceleration of the flow are observed from the modeling results which agree with the general experimental observation.

General information
State: Published
Organisations: CERE – Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Yuan, H. (Intern)
Number of pages: 228
Pages: 209-212
Publication date: 2010

Host publication information
Title of host publication: DTU Chemical Engineering Graduate School Yearbook 2009
Publisher: Technical University of Denmark, Department of Chemical Engineering
ISBN (Print): 978-87-92481-14-6
Main Research Area: Technical/natural sciences
elliptic, polydisperse, transport in porous media
Electronic versions:
yearbook15-12-2009.pdf
Source: orbit
Source-ID: 263788
Publication: Research › Book chapter – Annual report year: 2010

Phase equilibria modeling of methanol-containing systems with the CPA and sPC-SAFT equations of state

Proper representation at various conditions of phase equilibria of methanol-containing mixtures (with hydrocarbons, water, etc.) is important for oil flow assurance purposes. In this work two association equations of state, CPA and sPC-SAFT, are applied to methanol-containing mixtures. The purpose of this work is to investigate which association schemes (e.g. two-site, three-site) should be used for methanol which will result in successful representation of methanol-water-hydrocarbon phase equilibria. Parameters from the literature as well as newly estimated parameters based on vapor pressure, liquid density, enthalpy of vaporization and compressibility factor data are used. Successful representation of methanol-vapor-liquid equilibrium (VLE) and liquid-liquid equilibrium (LLE) data for methanol-water as well as water-methanol-hydrocarbon LLE are considered. It is concluded that the two association equations of state perform overall similarly, with the two-site association scheme being a better choice than the three-site scheme, for phase equilibrium calculations. Use of the additional properties (enthalpy of vaporization and compressibility factor) in the parameter estimation has a larger effect on the performance of sPC-SAFT compared to CPA (C) 2009 Elsevier B.V. All rights reserved

General information
State: Published
Organisations: CERE – Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, Technical University of Denmark
Authors: Tybjerg, P. C. V. (Ekstern), Kontogeorgis, G. (Intern), Michelsen, M. L. (Intern), Stenby, E. H. (Intern)
Pages: 128-138
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Journal: Fluid Phase Equilibria
Volume: 288
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BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
Potential of Economic Model Predictive Control for Management of Multiple Power Producers and Consumers

General information
State: Published
Organisations: Scientific Computing, Department of Informatics and Mathematical Modeling, Center for Energy Resources Engineering, DONG Energy A/S
Authors: Hovgaard, T. G. (Intern), Jørgensen, J. B. (Intern), Edlund, K. (Ekstern)
Publication date: 2010

Preparation and structural characterisation of novel and versatile amphiphilic octenyl succinic anhydride-modified hyaluronic acid derivatives
The purpose of the present study was to prepare amphiphilic hyaluronic acid (HA) derivatives and to study the influence of a selection of reaction parameters on the degree of substitution (DS) of the derivatives. Octenyl succinic anhydride (OSA)-modified HA (OSA–HA) derivatives were prepared and structurally characterised by Fourier transform-infrared spectroscopy and proton nuclear magnetic resonance spectroscopy (1H NMR). The influence of four reaction parameters on the DS of the derivatives was studied by means of an experimental design. The results showed that the OSA/HA molar ratio, the buffer (NaHCO3) concentration and their interaction had the largest influence while the HA concentration and the reaction time only had a negligible effect. According to 1H NMR the maximum DS achieved within the experimental conditions tested was 43% per disaccharide unit. Moreover optimal reaction conditions were identified for the preparation of versatile OSA–HA derivatives with a DS between 1.5% and 43%.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering, Novozymes A/S
Authors: Eenschooten, C. D. (Intern), Guillaumie, F. (Ekstern), Kontogeorgis, G. (Intern), Stenby, E. H. (Intern), Schwach-Abdellaoui, K. (Ekstern)
Pages: 597-605
Publication date: 2010
Main Research Area: Technical/natural sciences
Production Optimization for Two-Phase Flow in an Oil Reservoir

General information
State: Published
Organisations: Center for Energy Resources Engineering, Department of Informatics and Mathematical Modeling, Scientific Computing, Department of Chemistry
Authors: Völcker, C. (Intern), Jørgensen, J. B. (Intern), Thomsen, P. G. (Intern), Stenby, E. H. (Intern)
Publication date: 2010
Main Research Area: Technical/natural sciences
Electronic versions:
npcw10_abstract.pdf
Source: orbit
Source-ID: 268272
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2010

Refrigeration plants using carbon dioxide as refrigerant: measuring and modelling the solubility and diffusion of carbon dioxide in polymers used as sealing materials
Because of increased environmental pressure, there is currently a movement away from more traditional refrigerants such as HCFC's toward refrigerants with lower global warming potential such as carbon dioxide (CO2). However, the use of CO2 as a refrigerant requires a refrigeration cycle with greater extremes of pressure, placing greater demands on the polymer materials used for seals and packing. In this work we have measured the solubility and diffusivity of gaseous CO2 in two polymers used as sealing materials in CO2 refrigeration plants. These are Hydrogenated Nitrile Butadiene Rubber
(HNBR) and Ethylene Propylene Diene Monomer (EPDM) which are used in seals such as O-rings. The experiments were performed on a high-pressure microbalance. Solubility results were modelled using an equation of state for polymers (simplified PC-SAFT). The necessary polymer parameters were obtained using a previously published method. The measured results can be successfully correlated using simplified PC-SAFT.

**General information**

**State:** Published  
**Organisations:** CERE – Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering, Technical University of Denmark  
**Authors:** von Solms, N. (Intern), Kristensen, J. (Ekstern)  
**Pages:** 19-25  
**Publication date:** 2010  
**Main Research Area:** Technical/natural sciences

**Publication information**

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**Volume:** 33  
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- BFI (2018): BFI-level 1  
- Web of Science (2018): Indexed yes  
- BFI (2017): BFI-level 1  
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- Web of Science (2016): Indexed yes  
- BFI (2015): BFI-level 1  
- Scopus rating (2016): CiteScore 3.06 SJR 1.344 SNIP 1.598  
- Web of Science (2016): Indexed yes  
- BFI (2014): BFI-level 1  
- Scopus rating (2015): SJR 1.396 SNIP 1.537 CiteScore 2.44  
- Web of Science (2015): Indexed yes  
- BFI (2014): BFI-level 1  
- Scopus rating (2014): SJR 1.667 SNIP 2.117 CiteScore 2.6  
- Web of Science (2014): Indexed yes  
- BFI (2013): BFI-level 1  
- Scopus rating (2013): SJR 1.461 SNIP 1.979 CiteScore 2.25  
- ISI indexed (2013): ISI indexed yes  
- Web of Science (2013): Indexed yes  
- BFI (2012): BFI-level 1  
- Scopus rating (2012): SJR 1.426 SNIP 1.908 CiteScore 2.09  
- ISI indexed (2012): ISI indexed yes  
- Web of Science (2012): Indexed yes  
- BFI (2011): BFI-level 1  
- Scopus rating (2011): SJR 1.308 SNIP 2.129 CiteScore 2.2  
- ISI indexed (2011): ISI indexed yes  
- Web of Science (2011): Indexed yes  
- BFI (2010): BFI-level 1  
- Scopus rating (2010): SJR 1.372 SNIP 1.786  
- Web of Science (2010): Indexed yes  
- BFI (2009): BFI-level 1  
- Scopus rating (2009): SJR 1.569 SNIP 1.954  
- Web of Science (2009): Indexed yes  
- BFI (2008): BFI-level 1  
- Scopus rating (2008): SJR 1.309 SNIP 1.737  
- Web of Science (2008): Indexed yes  
- Scopus rating (2007): SJR 0.841 SNIP 1.646  
- Scopus rating (2006): SJR 1.5 SNIP 1.629  
- Scopus rating (2005): SJR 1.409 SNIP 1.718
Review and recommended thermodynamic properties of FeCO₃
An extensive review of entropy, enthalpy of formation and Gibbs energy of formation, heat capacity, aqueous solubility and solubility constant of FeCO₃ is given. A consistent set of thermodynamic properties for FeCO₃ and relevant aqueous species is selected and recommended for use. Speciation schemes for aqueous FeCO₃ are reviewed and evaluated. Issues related to supersaturation of FeCO₃ are discussed. Works on the thermal decomposition of FeCO₃ are presented and an overview of measured solubility and synthesis of FeCO₃ is given.

General information
State: Published
Organisations: CERE – Center for Energy Resourses Engineering, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Fosbøl, P. L. (Intern), Thomsen, K. (Intern), Stenby, E. H. (Intern)
Pages: 115-135
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Main Research Area: Technical/natural sciences

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Volume: 45
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BFI (2018): BFI-level 1
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Web of Science (2017): Indexed Yes
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Scopus rating (2016): CiteScore 0.86 SJR 0.382 SNIP 0.588
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.345 SNIP 0.673 CiteScore 0.92
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.38 SNIP 0.885 CiteScore 0.89
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.335 SNIP 0.608 CiteScore 0.62
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.284 SNIP 0.642 CiteScore 0.62
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.411 SNIP 1.058 CiteScore 0.72
ISI indexed (2011): ISI indexed yes
Review of the Upper Jurassic-Lower Cretaceous stratigraphy in Western Cameros basin, Northern Spain

The Upper Jurassic-Lower Cretaceous stratigraphy of the Cameros basin has been reviewed. In Western Cameros the stratigraphic sections are condensed but they have a parallel development with the basin depocentre and the same groups have been identified. The Tera Group consists of two formations: Señora de Brezales and Magaña. The Oncala Group is represented by two formations of fluvial deposits, Jaramillo de la Fuente and Río del Salcedal and a third formation, Rupelo of lacustrine/coastal carbonates and evaporites. The Peñacobia Formation is an independent formation made of biogenic lacustrine carbonates and it is restricted to SW Cameros. The Urbión Group is represented by the Laguna Negra Formation which is the deposit of a gravelly braidplain and occurs in NW Cameros and South Demanda. The Enciso Group encompasses three formations, Río Ciruelos which is made of fluvial deposits, Hortigüela which consists of fresh water lacustrine carbonates and Golmayo representing a fluvial dominated coastal plain with marly lakes. The Oliván Group encompasses three formations of fluvial deposits: La Gallega, Castrillo de la Reina and Cuerda del Pozo. The Salas Group consists of two formations Cabezón de la Sierra and Abejar of fluvial and aeolian deposits. The basin wide distribution of the Groups evidences the synchronous development of the rifting process across the basin and supports a model of a basin compartmentalised into multiple sectors evolving simultaneously under different rates of subsidence and terrigenous supply. The onlap of the syn-rift mega-sequence on the basin margins, the extra-basinal fluvial systems and shallow carbonate lakes together with its condensed character and the preservation of pre-rift mega-sequence at the basin margins point towards a basin with low-gradient basin margins.

General information
State: Published
Organisations: Section for Geotechnics and Geology, Department of Civil Engineering, Center for Energy Resources Engineering
Authors: Vidal, M. D. P. C. (Intern)
Pages: 101-143
Publication date: 2010
Main Research Area: Technical/natural sciences

Publication information
Journal: Sociedad Geologica de Espana. Revista
Volume: 23
Issue number: 2-3
ISSN (Print): 0214-2708
Ratings: Web of Science (2018): Indexed yes
Robust model identification applied to type 1 diabetes
In many realistic applications, process noise is known to be neither white nor normally distributed. When identifying models in these cases, it may be more effective to minimize a different penalty function than the standard sum of squared errors (as in a least-squares identification method). This paper investigates model identification based on two different penalty functions: the 1-norm of the prediction errors and a Huber-type penalty function. For data characteristic of some realistic applications, model identification based on these latter two penalty functions is shown to result in more accurate estimates of parameters than the standard least-squares solution, and more accurate model predictions for test data. The identification techniques are demonstrated on a simple toy problem as well as a physiological model of type 1 diabetes.

Rock physics model of glauconitic greensand from the North Sea

Sampling informative/complex a priori probability distributions using Gibbs sampling assisted by sequential simulation
Markov chain Monte Carlo methods such as the Gibbs sampler and the Metropolis algorithm can be used to sample the solutions to non-linear inverse problems. In principle these methods allow incorporation of arbitrarily complex a priori information, but current methods allow only relatively simple priors to be used. We demonstrate how sequential simulation
can be seen as an application of the Gibbs sampler, and how such a Gibbs sampler assisted by sequential simulation can be used to perform a random walk generating realizations of a relatively complex random function. We propose to combine this algorithm with the Metropolis algorithm to obtain an efficient method for sampling posterior probability densities for nonlinear inverse problems.
Systematic Model Analysis for Single Cell Protein (SCP) Production in a U-Loop Reactor

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, Scientific Computing, Department of Informatics and Mathematical Modeling, Center for Energy Resources Engineering
Authors: Prado Rubio, O. A. (Intern), Jørgensen, J. B. (Intern), Jørgensen, S. B. (Intern)
Pages: 319-324
Publication date: 2010

Host publication information
Title of host publication: Computer-Aided Chemical Engineering Series
Volume: Volume 28
Main Research Area: Technical/natural sciences
Conference: 20th European Symposium on Computer Aided Process Engineering, Ischia, Italy, 06/06/2010 - 06/06/2010
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Source-ID: 255425
Publication: Research - peer-review › Article in proceedings – Annual report year: 2010

The Potential of Economic MPC for Power Management
Economic Model Predictive Control is a receding horizon controller that minimizes an economic objective function rather than a weighted least squares objective function as in Model Predictive Control (MPC). We use Economic MPC to operate a portfolio of power generators and consumers such that the cost of producing the required power is minimized. The power generators are controllable power generators such as combined heat and power generators (CHP), coal and gas fired power generators, as well as a significant share of uncontrollable power generators such as parks of wind turbines. In addition, some of the power consumers are controllable. In this paper, the controllable power consumers are exemplified by large cold rooms or aggregations of super markets with refrigeration systems. We formulate the Economic MPC as a linear program. By simulation, we demonstrate the performance of Economic MPC for a small conceptual example.

General information
State: Published
Organisations: Scientific Computing, Department of Informatics and Mathematical Modeling, Center for Energy Resources Engineering, DONG Energy A/S
Authors: Hovgaard, T. G. (Intern), Edlund, K. (Ekstern), Jørgensen, J. B. (Intern), Jørgensen, S. B. (Intern)
Pages: 7533-7538
Publication date: 2010

Host publication information
Tilting oil-water contact in the chalk of Tyra Field as interpreted from capillary pressure data
The Tyra Field in the central North Sea is located in Palaeogene and Upper Cretaceous chalk. It contains a natural gas zone underlain by an oil leg. Based on analysis of logs and core data from ten wells drilled prior to the field being put into production, normalized water saturation depth-trends from logs were compared with normalized water saturation depth-trends predicted from capillary pressure core data. The ten wells lie close to a SW–NE cross section of the field. For the gas–oil contact, a free contact measured in one well corresponds to a practically horizontal contact interpreted from logging data in the remaining wells. A westerly dipping oil–water contact was found from logging data. Comparison of the depth-wise trends in normalized water saturation among the different wells indicates a regional pattern: in the western side of the field, the trends correspond to a situation of imbibition, where the free water level overlies an interval of residual oil, whereas in the eastern part of the field, the depth-wise trends in normalized water saturation correspond to a situation of drainage. The free water level apparently dips to the east due either to hydrodynamic action or to pressure inequilibrium in the aquifer following tectonic tilting.

Transport of reservoir fines: a novel model for formation heterogeneity and particle heterogeneity
Modeling transport of reservoir fines is of great importance for evaluating the damage of production wells and infectivity decline. The conventional methodology accounts for neither the formation heterogeneity around the wells nor the reservoir fines’ heterogeneity. We have developed an integral model incorporating the elliptic equation based on continuous time random walk and distributed filtration coefficients, respectively reflecting the influences of the formation heterogeneity around the wells and the reservoir fines’ heterogeneity. The novel methodology excels the classical advection dispersion equation in modeling the transport and the deposition of reservoir fines. It successfully predicts the unsymmetrical concentration profiles and the hyperexponential deposition in experiments.
Tuning of ARX-based Model Predictive Control for Offset-free Tracking

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Mathematical Statistics, Department of Informatics and Mathematical Modeling, Computer Aided Process Engineering Center, Scientific Computing, Center for Energy Resources Engineering
Authors: Huusom, J. K. (Intern), Poulsen, N. K. (Intern), Jørgensen, S. B. (Intern), Jørgensen, J. B. (Intern)
Publication date: 2010

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Tuning of ARX-based Model Predictive Control for Offset-free Tracking

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Mathematical Statistics, Department of Informatics and Mathematical Modeling, Computer Aided Process Engineering Center, Scientific Computing, Center for Energy Resources Engineering
Authors: Huusom, J. K. (Intern), Poulsen, N. K. (Intern), Jørgensen, S. B. (Intern), Jørgensen, J. B. (Intern)
Publication date: 2010

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
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Publication: Research › Article in proceedings – Annual report year: 2010

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Title of host publication: Proceedings of Dansk Kemiingeniørkonference 2010
Main Research Area: Technical/natural sciences
Conference: 3. Dansk KemiingeniørKonference, Kgs. Lyngby, Denmark, 16/06/2010 - 16/06/2010
Source: orbit
Source-ID: 266242
Publication: Research › Article in proceedings – Annual report year: 2010

Tuning of ARX-based Model Predictive Control for Offset-free Tracking

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Mathematical Statistics, Department of Informatics and Mathematical Modeling, Computer Aided Process Engineering Center, Scientific Computing, Center for Energy Resources Engineering
Tuning of methods for offset free MPC based on ARX model representations

In this paper we investigate model predictive control (MPC) based on ARX models. ARX models can be identified from data using convex optimization technologies and is linear in the system parameters. Compared to other model parameterizations this feature is an advantage in embedded applications for robust and automatic system identification. Standard MPC is not able to reject a sustained, unmeasured, non zero mean disturbance and will therefore not provide offset free tracking. Offset free tracking can be guaranteed for this type of disturbances if Δ variables are used or if the state space is extended with a disturbance model state. The relation between the base case and the two extended methods are illustrated which provides good understanding and a platform for discussing tuning for good closed loop performance.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Mathematical Statistics, Department of Informatics and Mathematical Modeling, Computer Aided Process Engineering Center, Scientific Computing, Center for Energy Resources Engineering
Authors: Huusom, J. K. (Intern), Poulsen, N. K. (Intern), Jørgensen, S. B. (Intern), Jørgensen, J. B. (Intern)
Pages: 2255-2360
Publication date: 2010

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Publisher: IEEE
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Main Research Area: Technical/natural sciences
Conference: American Control Conference (ACC 2010), Baltimore, MD, United States, 03/06/2010 - 03/06/2010
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Tuning of Offset-Free ARX-based SISO Model Predictive Control

General information
State: Submitted
Organisations: Department of Chemical and Biochemical Engineering, Mathematical Statistics, Department of Informatics and Mathematical Modeling, Computer Aided Process Engineering Center, Scientific Computing, Center for Energy Resources Engineering
Authors: Huusom, J. K. (Intern), Poulsen, N. K. (Intern), Jørgensen, S. B. (Intern), Jørgensen, J. B. (Intern)
Publication date: 2010

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Conference: IEEE Conference on Decision and Control, Atlanta, Georgia, USA, 01/01/2010
Source: orbit
Source-ID: 264877
Publication: Research - peer-review › Article in proceedings – Annual report year: 2010

Water weakening of chalk explained from a fluid-solid friction factor
The hypothesis behind this paper proposal is that the Biot critical frequency can be used to characterize the water weakening phenomenon physically. The Biot critical frequency determines the transition from where an applied sound
velocity on a saturated porous chalk is dominated by viscous forces to where it is dominated by inertial forces, i.e. when the pore fluid motion lags behind the applied frequency. It is therefore a measure of the internal surface friction between solid and fluid which can be interpreted as a friction factor on the pore scale and we propose it can be extrapolated to the macroscale failure and pore collapse properties. The Biot critical frequency incorporates the porosity, permeability, fluid density and fluid viscosity, where the latter is highly temperature dependent – it does not include the applied sound velocity frequency. The listed parameters are usually determined during laboratory tests and the fluid viscosity and density may be found in tabulated references. There exist a number of previously published laboratory test results on chalk which was collected from Brazilian, unconfined compression and triaxial tests. The data spans four different chalk types which were tested at temperatures from 20°C to 130°C with the following pore fluids: fresh water, synthetic seawater of different chemical compositions, methanol, glycol, and oil of varying viscosity. The data was evaluated according to failure lines and yield envelopes for all fluids and temperatures while using the Biot critical frequency as a single reference. Other viscoplastic parameters were investigated in the same manner to verify the range of the functioning of the friction factor. The findings show that the Biot critical frequency can be used as a common friction factor and is useful in combining laboratory results. It is also inferred that the observed water weakening phenomenon may be attributed to the friction between solid and fluid.

General information
State: Published
Organisations: Section for Geotechnics and Geology, Department of Civil Engineering, Department of Environmental Engineering, Center for Energy Resources Engineering
Authors: Andreassen, K. A. (Intern), Fabricius, I. L. (Intern)
Pages: 26-35
Publication date: 2010

Host publication information
Title of host publication: Rock Mechanics in the Nordic Countries 2010
Volume: Proceedings-DVD
Main Research Area: Technical/natural sciences
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Source: orbit
Source-ID: 270970
Publication: Research - peer-review › Article in proceedings – Annual report year: 2010

Analysis and applications of a group contribution sPC-SAFT equation of state
A group contribution (GC) method for estimating pure compound parameters for the molecular-based perturbed-chain statistical associating fluid theory (PC-SAFT) equation of state (EoS) is proposed in a previous work [A. Tihic, G.M. Kontogeorgis, N. von Solms, M.L Michelsen, L Constantinou. Ind. Eng. Chem. Res. 47 (2008) 5092-5101]. In this paper, an investigation of the predictive capability of the CC sPC-SAFT EoS through comparison of the method's predictions for compounds with high molecular weights and several selected binary mixtures of industrial significance with experimental data such as thiols, sulphides and polynuclear aromatics is presented. Additionally, predictions of activity coefficient at infinite dilution for athermal systems are compared with the results using existing activity coefficient models. The results show that calculated pure compound parameters using the proposed CC method allow satisfactory representation of experimental data of investigated systems with the sPC-SAFT EoS. Moreover, the variety of functional groups in the available GC scheme ensures broad applications of the CC sPC-SAFT EoS.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Phase Equilibria and Separation Processes, Center for Energy Resources Engineering
Authors: Tihic, A. (Intern), von Solms, N. (Intern), Michelsen, M. L. (Intern), Kontogeorgis, G. (Intern), Constantinou, L. (Ekstern)
Pages: 60-69
Publication date: 2009
Main Research Area: Technical/natural sciences

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Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
Application of sPC-SAFT and group contribution sPC-SAFT to polymer systems—Capabilities and limitations

A group contribution (GC) version of the simplified Perturbed-Chain Statistical Associating Fluid Theory (sPC-SAFT) Equation of State is proposed in a previous work [A. Tihic, G.M. Kontogeorgis, N. von Solms, M.L. Michelsen, L Constantinou, Ind. Eng. Chem. Res. 47 (2008) 5092-5101]. The reported predictive capability of the model demonstrates satisfactory description of the fluid behaviour of several polymer systems, including both vapour-liquid equilibria and liquid-liquid equilibria. This work continues the systematic study on phase behaviour of polymer systems with the two versions of the sPC-SAFT model, with and without GC. The reported results contribute to a better understanding of the applicability of the sPC-SAFT model to binary polymer mixtures, and identify both models as good predictive tools for several industrial applications. Limitations are also identified and discussed.
Application of the CPA equation of state to reservoir fluids in presence of water and polar chemicals

The complex phase equilibrium between reservoir fluids and associating compounds like water, methanol and glycols has become more and more important as the increasing global energy demand pushes the oil industry to target reservoirs with extreme or complicated conditions, such as deep or offshore reservoirs. Conventional equation of state (EoS) with classical mixing rules cannot satisfactorily predict or even correlate the phase equilibrium of those systems. A promising model for such systems is the Cubic-Plus-Association (CPA) EoS, which has been successfully applied to well-defined systems containing associating compounds. In this work, a set of correlations was proposed to calculate the CPA model parameters for the narrow cuts in ill-defined C7+ fractions. The correlations were then combined with either the characterization method of Pedersen et al. or that of Whitson et al. to extend CPA to reservoir fluids in presence of water and polar chemical such as methanol and monoethylene glycol. With a minimum number of adjustable parameters from binary pairs, satisfactory results have been obtained for different types of phase equilibria in reservoir fluid systems and several relevant model multicomponent systems. In addition, modeling of mutual solubility between light hydrocarbons and water is also addressed.

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Yan, W. (Intern), Kontogeorgis, G. (Intern), Stenby, E. H. (Intern)
Pages: 75-85
Publication date: 2009
Main Research Area: Technical/natural sciences

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C7+ characterization, Reservoir fluid, Equation of state, Polar chemical, Water

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Challenges in Teaching 'Colloid and Surface Chemistry' -- A Danish Experience

General information
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Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, The Danish Polymer Centre, Center for Energy Resources Engineering
Authors: Kontogeorgis, G. (Intern), Vigild, M. E. (Intern)
Pages: 137-142
Publication date: 2009
Main Research Area: Technical/natural sciences

Publication information
Journal: Chemical Engineering Education
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Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 0.141 SNIP 0.468 CiteScore 0.3
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.555 SNIP 0.74 CiteScore 0.41
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.672 SNIP 0.959 CiteScore 0.52
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.549 SNIP 0.805 CiteScore 0.42
ISI indexed (2013): ISI indexed no
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.353 SNIP 0.638 CiteScore 0.38
ISI indexed (2012): ISI indexed no
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.301 SNIP 1.018 CiteScore 0.43
ISI indexed (2011): ISI indexed no
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.419 SNIP 0.631
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.4 SNIP 0.616
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.543 SNIP 0.869
Scopus rating (2007): SJR 0.502 SNIP 0.413
Scopus rating (2006): SJR 0.345 SNIP 0.629
Scopus rating (2005): SJR 0.247 SNIP 0.607
Scopus rating (2004): SJR 0.747 SNIP 0.851
Scopus rating (2003): SJR 1.701 SNIP 1.066
Scopus rating (2002): SJR 1.378 SNIP 1.428
Scopus rating (2001): SJR 0.914 SNIP 0.856
Scopus rating (2000): SJR 0.486 SNIP 0.649
Scopus rating (1999): SJR 0.23 SNIP 0.867
Original language: English
Source: orbit
Source-ID: 211602
Publication: Research - peer-review › Journal article – Annual report year: 2009
Chilled ammonia process for CO2 capture

The chilled ammonia process absorbs the CO2 at low temperature (2-10 degrees C). The heat of absorption of carbon dioxide by ammonia is significantly lower than for amines. In addition, degradation problems can be avoided and a high carbon dioxide capacity is achieved. Hence, this process shows good perspectives for decreasing the energy requirement. However, a scientific understanding of the processes is required. The properties of the NH3-CO2-H2O system were described using the Extended UNIQUAC electrolyte model developed by Thomsen and Rasmussen in a temperature range from 0 to 110 degrees C and pressure up to 100 bars [1]. The results show that solid phases consisting of ammonium carbonate and bicarbonate are formed in the absorber. The energy requirements in the absorber and in the desorber have been studied. The enthalpy calculations show that an energy requirement for the desorber lower than 2 GJ/ton CO2 can be reached. (c) 2008 Elsevier Ltd. All rights reserved.

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Darde, V. C. A. (Intern), Thomsen, K. (Intern), van Well, W. J. M. (Ekstern), Stenby, E. H. (Intern)
Pages: 1035-1042
Publication date: 2009

Host publication information
Title of host publication: GREENHOUSE GAS CONTROL TECHNOLOGIES 9
Publisher: Elsevier
Series: Energy Procedia
Volume: 1
Number: 1
ISSN: 1876-6102
Main Research Area: Technical/natural sciences
DOIs: 10.1016/j.egypro.2009.01.137
Source: orbit
Source-ID: 262133
Publication: Research - peer-review › Article in proceedings – Annual report year: 2009

CO2 Capture and Storage Projects at IVC-SEP

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Fosbøl, P. L. (Intern)
Publication date: 2009
Event: Poster session presented at DTU åbent hus, Technical University of Denmark, DTU, Lyngby, Denmark,
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 255524
Publication: Research › Poster – Annual report year: 2009

CO2 Capture from Flue Gas using Amino Acid Salt Solutions

The reversible absorption of CO2 into a chemical solvent is currently the leading CO2 capture technology. Available solvents are almost exclusively based on aqueous alkanolamine solutions, which entail both economic and environmental complications, making the commercialization of the technology difficult. Amino acid salt solutions have emerged as an alternative to the alkanolamine solutions. A number of advantages make amino acid salt solutions attractive solvents for CO2 capture from flue gas. In the present study CO2 absorption in aqueous solutions of 0.5 M potassium glycinate and 0.5 M monoethanolamine (MEA) were performed, using a stirred cell reactor experimental setup. The absorption of gas containing 10 mol % CO2 and 90 mol % N2 was followed by measuring the percentage of CO2 in the outlet gas. Also the temperature and pH in the solutions were measured during the absorption. The results showed that the CO2 absorption curves of potassium glycinate and MEA are very similar indicating a potential for potassium glycinate as replacement for MEA in chemical absorption of CO2 from flue gas. For both the potassium glycinate and the MEA solutions the CO2 loading capacity was 0.8 mol CO2/mol amine and the pH dropped between 2 and 3 units during the absorption process. In both types of solutions the temperature increased as a result of the CO2 absorption, which is expected due to the exothermic nature of the absorption reaction. The increase in temperature for the potassium glycinate was lower than for
MEA indicating a lower heat of absorption/desorption.

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Lerche, B. M. (Intern), Stenby, E. H. (Intern), Thomsen, K. (Intern)
Pages: 233-241
Publication date: 2009

Host publication information
Title of host publication: Energy solutions for CO2 emission peak and subsequent decline. Proceedings
Publisher: Danmarks Tekniske Universitet, Risø Nationallaboratoriet for Bæredygtig Energi
Main Research Area: Technical/natural sciences
Electronic versions:
content.pdf
Links:

Bibliographical note
Rise-R-1712(EN)
Source: orbit
Source-ID: 255417
Publication: Research - peer-review › Article in proceedings – Annual report year: 2009

CURRICULUM - Teaching Chemical Engineering Thermodynamics at Three Levels: Experience from the Technical University of Denmark

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Center for Energy Resources Engineering
Authors: Kontogeorgis, G. (Intern), Michelsen, M. L. (Intern), Clement, K. (Intern)
Pages: 70-78
Publication date: 2009
Main Research Area: Technical/natural sciences

Publication information
Journal: Chemical Engineering Education
Volume: 43
Issue number: 1
ISSN (Print): 0009-2479
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 0.141 SNIP 0.468 CiteScore 0.3
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.555 SNIP 0.74 CiteScore 0.41
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.672 SNIP 0.959 CiteScore 0.52
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.549 SNIP 0.805 CiteScore 0.42
ISI indexed (2013): ISI indexed no
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.353 SNIP 0.638 CiteScore 0.38
ISI indexed (2012): ISI indexed no
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.301 SNIP 1.018 CiteScore 0.43
ISI indexed (2011): ISI indexed no
Electrodeposition of Asphaltenes. 1. Preliminary Studies on Electrodeposition from Oil-Heptane Mixtures

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Khvostichenko, D. (Intern), Andersen, S. I. (Intern)
Pages: 811-819
Publication date: 2009
Main Research Area: Technical/natural sciences

Publication Information
Journal: Energy & Fuels
Volume: 23
Issue number: 2
ISSN (Print): 0887-0624
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.49
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 3.34
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 3.3
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 3.52
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 3.25
ISI indexed (2012): ISI indexed yes
Energy Demand for CO2 Solvent Regeneration

**General information**
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Fosbøl, P. L. (Intern), Thomsen, K. (Intern), Stenby, E. H. (Intern)
Pages: 242-252
Publication date: 2009

**Host publication information**
Title of host publication: Energy solutions for CO2 emission peak and subsequent decline. Proceedings
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 245519
Publication: Research - peer-review › Journal article – Annual report year: 2009

Estimation of the Impact of Sulfur Species on Glycol Dehydration

**General information**
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Afzal, W. (Intern), Breil, M. P. (Intern), Mohammadi, A. H. (Ekstern), Kontogeorgis, G. (Intern), Richon, D. (Ekstern)
Number of pages: 23
Publication date: 2009

**Host publication information**
Title of host publication: Book of abstracts: Equifase 2009
Main Research Area: Technical/natural sciences
The extended UNIQUAC model [K. Thomsen, R Rasmussen, Chem. Eng. Sci. 54 (1999) 1787-1802] was applied to the thermodynamic representation of carbon dioxide absorption in aqueous monoethanolamine (MEA), methyldiethanolamine (MDEA) and varied strength mixtures of the two alkanolamines (MEA-MDEA). For these systems, altogether 13 interaction model parameters are adjusted. Out of these parameters, 11 are temperature dependent. All the essential parameters of the model are simultaneously regressed to a collective set of data on the single MEA and MDEA systems. Different types of data are used for modeling and they cover a very wide range of conditions. Vapor-liquid equilibrium (VLE) data for the aqueous alkanolamine systems containing CO2 in the pressure range of 3-13,000 kPa and temperatures of 25-200 C are used. The model is also regressed with the VLE and freezing point depression data of the binary aqueous alkanolamine systems (MEA-water and MDEA-water). The two just mentioned types of data cover the full concentration range of alkanolamines from extremely dilute to almost pure. The experimental freezing point depression data down to the temperature of -20 degrees C are used. Experimental excess enthalpy (H-E) data of the binary MEA-water and MDEA-water systems at 25, 40, 65 and 69 degrees C are used as well. In order to enhance the calculation of the infinite dilution activity coefficients of MEA and MDEA, the pure alkanolamines vapor pressure data in a relevant temperature range (up to almost 230 degrees C) are included in the parameter estimation process. The previously unavailable standard state properties of the alkanolamine ions appearing in this work, i.e. MEA protonate, MEA carbamate and MDEA protonate are determined. The concentration of the species in both MEA and MDEA solutions containing CO2 are predicted by the model and in the case of MEA compared to NMR spectroscopic data.
Improving Mechanistic CO2 Corrosion Models

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Fosbøl, P. L. (Intern), Thomsen, K. (Intern), Stenby, E. H. (Intern)
Publication date: 2009

Host publication information
Title of host publication: Proceedings CORROSION/09
Volume: Paper no. 09561
Publisher: National Association of Corrosion Engineers
Main Research Area: Technical/natural sciences
Conference: CORROSION 2009 : NACE Conference, Atlanta, Georgia, USA, 01/01/2009
Source: orbit
Source-ID: 239780
Publication: Research - peer-review › Article in proceedings – Annual report year: 2009

Interactions between Mica Surfaces across Crude Oil and Asphaltene Solutions

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Khvostichenko, D. (Intern), Andersen, S. I. (Intern)
Pages: 3660-3665
Publication date: 2009
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Physical Chemistry Part C: Nanomaterials and Interfaces
Volume: 113
Issue number: 9
ISSN (Print): 1932-7447
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 4.48 SJR 1.948 SNIP 1.181
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.917 SNIP 1.268 CiteScore 4.68
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 2.027 SNIP 1.448 CiteScore 5.08
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 2.134 SNIP 1.439 CiteScore 5.14
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 2.514 SNIP 1.46 CiteScore 4.98
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Modeling adsorption of liquid mixtures on porous materials

The multicomponent potential theory of adsorption (MPTA), which was previously applied to adsorption from gases, is extended onto adsorption of liquid mixtures on porous materials. In the MPTA, the adsorbed fluid is considered as an inhomogeneous liquid with thermodynamic properties that depend on the distance from the solid surface (or position in the porous space). The theory describes the two kinds of interactions present in the adsorbed fluid, i.e. the fluid-fluid and fluid-solid interactions, by means of an equation of state and interaction potentials, respectively. The proposed extension of the MPTA onto liquids has been tested on experimental binary and ternary adsorption data. We show that, for the set of experimental data considered in this work, the MPTA model is capable of correlating binary adsorption equilibria. Based on binary adsorption data, the theory can then predict ternary adsorption equilibria. Good agreement with the theoretical predictions is achieved in most of the cases. Some limitations of the model are also discussed.

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Monsalvo, M. A. (Intern), Shapiro, A. (Intern)
Pages: 310-316
Publication date: 2009
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Colloid and Interface Science
Volume: 333
Issue number: 1
ISSN (Print): 0021-9797
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 4.14 SJR 1.144 SNIP 1.267
Modeling of the Migration of Glycerol Monoester Plasticizers in Highly Plasticized Poly(vinyl chloride)

Different migration models were evaluated on the basis of data from migration experiments carried out by Danisco in 2005. The migration experiments were set up to investigate the behavior of the three plasticizers GRINDSTED (R) SOFT-
N-SAFE (SNS), GRINDSTED (R) ACETEM 95 CO (Acetem), and epoxidized soybean oil (ESBO) with regard to their migration from three different types of poly(vinyl chloride) into isooctane at 20, 40, and 60 degrees C. Diffusion coefficients derived from the experimental migration data were evaluated against diffusion coefficients estimated from a model based solely on the migration data for ESBO. The diffusion coefficient estimation model proved to be very good in estimating the diffusion coefficients at 20 degrees C but overestimated them at 40 degrees C and 60 degrees C. By using a migration model originally derived by Kontominas [Kondyli et al., Polymer, 34,2592 (1993)] and the estimated diffusion coefficients, it was possible to obtain a more satisfactory representation of the experimental migration data at 40 degrees C than that obtained with the commonly used migration model of Crank [Crank, Mathematics of diffusion, (1956)] based on the experimental diffusion coefficients. J. VINYL ADDIT. TECHNOL., 15:147-158, 2009. (C) 2009 Society of Plastics Engineers
Modeling of the Mixed Solvent Electrolyte System CO2-Na2CO3-NaHCO3-Monoethylene Glycol-Water
The extended UNIQUAC electrolyte activity coefficient model has been correlated to 751 experimental solid–liquid equilibrium (SLE), vapor–liquid equilibrium (VLE), and excess enthalpy data for the mixed solvent CO2–NaHCO3–Na2CO3–monoethylene glycol(MEG)–H2O electrolyte system. The model was validated by predicting the excess heat capacity. The model is consistent, and one set of binary interaction parameters are used for calculating all the properties between −50 and 90 °C. The model is compared to experimental data of infinite dilution activity coefficient measurements of MEG and may be used for calculating activities, solubility, salt hydrate properties, pH, and CO2 solubility in the NaHCO3–Na2CO3–MEG–H2O system. A simple density model of NaHCO3–Na2CO3–NaCl–MEG–water is given.

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Fosbøl, P. L. (Intern), Thomsen, K. (Intern), Stenby, E. H. (Intern)
Pages: 4565-4578
Publication date: 2009
Main Research Area: Technical/natural sciences

Publication information
Journal: Industrial & Engineering Chemistry Research
Volume: 48
Issue number: 9
ISSN (Print): 0888-5885
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.1 SJR 0.945 SNIP 1.139
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.949 SNIP 1.146 CiteScore 2.87
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.012 SNIP 1.292 CiteScore 2.85
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 0.982 SNIP 1.243 CiteScore 2.6
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.066 SNIP 1.338 CiteScore 2.56
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.086 SNIP 1.24 CiteScore 2.58
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
Modeling the Phase Behavior in Mixtures of Pharmaceuticals with Liquid or Supercritical Solvents

The concept of solubility parameter, which is widely used for the screening of solvents in pharmaceutical applications, is combined with a thermodynamic theory that is able to model systems with large deviations from ideal behavior. The nonrandom hydrogen-bonding (NRHB) theory is applied to model the phase behavior of mixtures of six pharmaceuticals (i.e., ibuprofen, ketoprofen, naproxen, benzoic acid, methyl paraben, and ethyl paraben). The pure fluid parameters of the studied pharmaceuticals were estimated using limited available experimental (or predicted) data on sublimation pressures, liquid densities, and Hansen’s solubility parameters. The complex hydrogen-bonding behavior was explicitly accounted for, while the corresponding parameters were adopted from simpler molecules of similar chemical structure or/and fitted to the aforementioned pure fluid properties. In this way, the solubility of the studied pharmaceuticals in liquid solvents was calculated. The average root-mean-square deviation between experimental and calculated solubilities is 0.190 and 0.037 in log10 units for prediction (calculations without a binary interaction parameter adjustment) and for correlation (calculations using one binary interaction parameter fitted to experimental data), respectively. In addition, using one temperature-independent binary interaction parameter the phase behavior of pharmaceuticals in supercritical CO2 and ethane was satisfactorily correlated. Finally, preliminary encouraging results are shown concerning two ternary mixtures where the model is able to predict accurately the solubility of pharmaceuticals in mixed solvents based on interaction parameters fitted to corresponding single solvent data.

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Tsivintzelis, I. (Intern), Economou, I. (Intern), Kontogeorgis, G. (Intern)
Pages: 6446-6458
Publication date: 2009
Main Research Area: Technical/natural sciences
Modeling the Solid-Liquid Equilibrium in Pharmaceutical-Solvent Mixtures: Systems with Complex Hydrogen Bonding Behavior

A methodology is suggested for modeling the phase equilibria of complex chemical mixtures with an equation of state (EoS) for the case where only limited experimental data exist. The complex hydrogen bonding behavior is explicitly accounted for and the corresponding parameters are adopted from simpler molecules of similar chemical structure and/or are fitted to Hansen's partial solubility parameters. The methodology is applied to modeling the solubility of three pharmaceuticals, namely acetanilide, phenacetin, and paracetamol, using the nonrandom hydrogen bonding (NRHB) EoS. In all cases, accurate correlations were obtained. The prediction ability of the approach was evaluated against predictions from the COSMO-RS model. A thorough discussion is made for the appropriate modeling of solid solubility considering the effect of the difference of the heat capacities of the solute in liquid and solid state, \( \Delta C_p = C_p - C_{ps} \), in the determination of solid chemical potential and, also, of the polymorphism of drugs.

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Tsivintzelis, I. (Intern), Economou, I. (Intern), Kontogeorgis, G. (Intern)
Pages: 756-770
Publication date: 2009
Main Research Area: Technical/natural sciences

Publication information
Journal: A I Ch E Journal
Volume: 55
Issue number: 3
ISSN (Print): 0001-1541
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.11 SJR 1.034 SNIP 1.268
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.085 SNIP 1.417 CiteScore 3.03
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.07 SNIP 1.332 CiteScore 2.86
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.05 SNIP 1.364 CiteScore 2.59
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 0.989 SNIP 1.437 CiteScore 2.46
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Modeling the vapor-liquid equilibria of polymer-solvent mixtures: Systems with complex hydrogen bonding behavior

The vapor-liquid equilibria of binary polymer–solvent systems was modeled using the Non-Random Hydrogen Bonding (NRHB) model. Mixtures of poly(ethylene glycol), poly(propylene glycol), poly(vinyl alcohol) and poly(vinyl acetate) with various solvents were investigated, while emphasis was put on hydrogen bonding systems, in which functional groups of the polymer chain can self-associate or cross-associate with the solvent molecules. Effort has been made to explicitly account for all hydrogen bonding interactions. The results reveal that the NRHB model offers a flexible approach to account for various self- or cross-associating interactions. In most cases model's predictions (using no binary interaction parameter $k_{ij} = 0$) and model's correlations (using one temperature independent binary interaction parameter, $k_{ij} \neq 0$) are in satisfactory agreement with the experimental data, despite the complexity of the examined systems.

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Tsivintzelis, I. (Intern), Kontogeorgis, G. (Intern)
Pages: 100-109
Publication date: 2009
Main Research Area: Technical/natural sciences

Publication information
Journal: Fluid Phase Equilibria
Volume: 280
Ratings:

BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 2.33 SJR 0.869 SNIP 1.155
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.874 SNIP 0.998 CiteScore 1.99
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 0.982 SNIP 1.248 CiteScore 2.28
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.007 SNIP 1.274 CiteScore 2.31
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.152 SNIP 1.286 CiteScore 2.31
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.034 SNIP 1.234 CiteScore 2.26
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 0.986 SNIP 1.317
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.133 SNIP 1.164
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.227 SNIP 1.09
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.031 SNIP 1.151
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.034 SNIP 1.245
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.009 SNIP 1.3
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 0.985 SNIP 1.349
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 1.193 SNIP 1.301
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 0.722 SNIP 1.101
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 0.966 SNIP 1.284
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 0.87 SNIP 0.898
Web of Science (2000): Indexed yes
On the thermodynamics of the McMillan-Mayer state function

The osmotic second virial coefficient is a key parameter in light scattering, protein crystallisation, self-interaction chromatography, and osmometry. The interpretation of the osmotic second virial coefficient depends on the solution theory. On the macroscopic level an expansion of the osmotic pressure is employed. A common statistical interpretation of the osmotic second virial coefficient of the expansion employs the McMillan-Mayer framework and the potential of mean force to characterise the solute-solute interaction. Supplementary to the statistical interpretation, it may be advantageous to develop the McMillan-Mayer framework in a classical thermodynamic context for which we develop the relationship between the state function of the McMillan-Mayer framework and the Helmholtz state function. A Taylor expansion method can be applied to the osmotic pressure of a solution which is dilute with respect to at least one solute component. This offers the possibility for an interpretation and correlation of the osmotic second virial coefficient utilising a McMillan-Mayer state function derived from a Helmholtz state function.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Phase Equilibria and Separation Processes, Center for Energy Resources Engineering
Authors: Mollerup, J. (Intern), Breil, M. P. (Intern)
Pages: 18-23
Publication date: 2009
Main Research Area: Technical/natural sciences

Publication information
Journal: Fluid Phase Equilibria
Volume: 276
Issue number: 1
ISSN (Print): 0378-3812
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 2.33 SJR 0.869 SNIP 1.155
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.874 SNIP 0.998 CiteScore 1.99
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 0.982 SNIP 1.248 CiteScore 2.28
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.007 SNIP 1.274 CiteScore 2.31
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.152 SNIP 1.286 CiteScore 2.31
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.034 SNIP 1.234 CiteScore 2.26
ISI indexed (2011): ISI indexed yes
Phase Equilibria of Mixtures Containing Glycol and n-Alkanes: Experimental Study of Infinite Dilution Activity Coefficients and Modeling Using the Cubic-Plus-Association Equation of State

In this work, we report the infinite dilution activity coefficients for four n-alkanes (n-pentane, n-hexane, n-heptane, and n-octane) in monoethylene glycol in the temperature range from 298 to 334 K and at atmospheric pressure. Experimental data were measured using a previously described inert gas stripping technique. The new experimental data are compared with the literature data whenever possible. The experimental infinite dilution activity coefficients of several alkanes from n-
pentane to n-hexadecane in monoethylene glycol, diethylene glycol, triethylene glycol, and tetraethylene glycol previously reported in the literature, along with the data measured in this work have been modeled using the cubic-plus-association (CPA) equation of state (EoS). Satisfactory results have been obtained using temperature-independent interaction parameters. Useful remarks are presented about the application of infinite dilution activity coefficient data for estimating binary interaction parameters of the CPA EoS for the description of whole vapor–liquid equilibria. Furthermore, the variation in the values of the interaction parameters is discussed for different glycol systems.

**General information**
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
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Main Research Area: Technical/natural sciences

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- BFI (2018): BFI-level 2
- Web of Science (2018): Indexed yes
- BFI (2017): BFI-level 2
- Web of Science (2017): Indexed yes
- BFI (2016): BFI-level 2
- Scopus rating (2016): CiteScore 3.1 SJR 0.945 SNIP 1.139
- Web of Science (2016): Indexed yes
- BFI (2015): BFI-level 2
- Scopus rating (2015): SJR 0.949 SNIP 1.146 CiteScore 2.87
- Web of Science (2015): Indexed yes
- BFI (2014): BFI-level 2
- Scopus rating (2014): SJR 1.012 SNIP 1.292 CiteScore 2.85
- Web of Science (2014): Indexed yes
- BFI (2013): BFI-level 2
- Scopus rating (2013): SJR 0.982 SNIP 1.243 CiteScore 2.6
- ISI indexed (2013): ISI indexed yes
- Web of Science (2013): Indexed yes
- BFI (2012): BFI-level 2
- Scopus rating (2012): SJR 1.066 SNIP 1.338 CiteScore 2.56
- ISI indexed (2012): ISI indexed yes
- Web of Science (2012): Indexed yes
- BFI (2011): BFI-level 2
- Scopus rating (2011): SJR 1.086 SNIP 1.24 CiteScore 2.58
- ISI indexed (2011): ISI indexed yes
- Web of Science (2011): Indexed yes
- BFI (2010): BFI-level 2
- Scopus rating (2010): SJR 1.047 SNIP 1.165
- Web of Science (2010): Indexed yes
- BFI (2009): BFI-level 2
- Scopus rating (2009): SJR 1.002 SNIP 1.164
- Web of Science (2009): Indexed yes
- BFI (2008): BFI-level 2
- Scopus rating (2008): SJR 1.142 SNIP 1.267
- Web of Science (2008): Indexed yes
- Scopus rating (2007): SJR 1.105 SNIP 1.239
Reducing complexity of inverse problems using geostatistical priors

In a probabilistic formulation of inverse problems the solution can be given as a sample of the posterior probability distribution. All realizations retained in the posterior sample are consistent with both an assumed prior model and observed data. Some inverse problems are unsolvable, in that one can practically never hope to generate a posterior sample, others are just ‘difficult’ and require special methods to become tractable, while others again are easily solved.

We discuss how difficult nonlinear inverse problems can be handled such that their complexity, i.e. the time taken to obtain a posterior sample, can be reduced significantly using informed priors based on geostatistical models. We discuss two approaches to include such geostatistically based prior information. One is based on a parametric description of the prior likelihood that applies to 2-point based statistical models, and another approach makes use of conditional re-simulation to sample the prior that works for both 2-point and multiple point random models. The latter approach is shown to be superior in terms of computational efficiency. We quantify the information content given by a specific choice of prior model. This enables us to obtain a lower limit of, for example, the size of a grid cell in a grid-parametrized parameter space. The resulting decrease in effective dimension of the parameter space provides a much more efficient sampling of the posterior with orders of magnitude increase in computational efficiency.

Simulation of Two-Phase Flow in an Oil Reservoir using Adaptive High-Order Runge-Kutta based Time-Integration

General information
State: Published
Organisations: Scientific Computing, Department of Informatics and Mathematical Modeling, Department of Chemistry, Center for Energy Resources Engineering
Authors: Völcker, C. (Intern), Jørgensen, J. B. (Intern), Thomsen, P. G. (Intern), Stenby, E. H. (Intern)
Solubility Measurements in the Mixed Solvent Electrolyte System Na2CO3-NaHCO3-Monoethylene Glycol-Water

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Fosbøl, P. L. (Intern), Thomsen, K. (Intern), Stenby, E. H. (Intern)
Pages: 2218-2228
Publication date: 2009

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Journal: Industrial & Engineering Chemistry Research
Volume: 48
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BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.1 SJR 0.945 SNIP 1.139
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.949 SNIP 1.146 CiteScore 2.87
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.012 SNIP 1.292 CiteScore 2.85
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 0.982 SNIP 1.243 CiteScore 2.6
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.066 SNIP 1.338 CiteScore 2.56
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.086 SNIP 1.24 CiteScore 2.58
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.047 SNIP 1.165
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.002 SNIP 1.164
Web of Science (2009): Indexed yes
Study of high-pressure adsorption from supercritical fluids by the potential theory

The multicomponent potential theory of adsorption (MPTA), which has been previously used to study low-pressure adsorption of subcritical fluids, is extended to adsorption equilibria from supercritical fluids up to high pressures. The MPTA describes an adsorbed phase as an inhomogeneous fluid with thermodynamic properties that depend on the distance from the solid surface (or position in the porous space). The description involves the two kinds of interactions present in the adsorbed fluid, i.e. the fluid-fluid and fluid-solid interactions accounted for by means of an equation of state (EoS) and interaction potential functions, respectively. This makes it possible to generate the different MPTA models by combination of the relevant EoS/potentials. In the present work, the simplified perturbed-chain statistical associating fluid theory (sPC-SAFT) EoS is used for the thermodynamic description of both the adsorbed and the gas phases. We have also evaluated the performance of the classical Soave-Redlich-Kwong (SRK) EoS. The fluid-solid interactions are described by simple Dubinin-Radushkevich-Astakhov (DRA) potentials. In addition, we test the performance of the 10-4-3 Steele potential. It is shown that application of sPC-SAFT slightly improves the performance of the MPTA and that in spite of its simplicity, the DRA model can be considered as an accurate potential, especially, for mixture adsorption. We show that, for the sets of experimental data considered in this work, the MPTA is capable of predicting adsorption of pure components and binary mixtures in wide ranges of pressure and temperature. A good agreement with the theoretical predictions is achieved in most of the cases. The MPTA is capable to correctly describe complex physical behavior observed at supercritical/high-pressure conditions. Some limitations of the model are also discussed.
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 2.33 SJR 0.869 SNIP 1.155
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.874 SNIP 0.998 CiteScore 1.99
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 0.982 SNIP 1.248 CiteScore 2.28
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.007 SNIP 1.274 CiteScore 2.31
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.152 SNIP 1.286 CiteScore 2.31
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.034 SNIP 1.234 CiteScore 2.26
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 0.986 SNIP 1.317
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.133 SNIP 1.164
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.227 SNIP 1.09
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.031 SNIP 1.151
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.034 SNIP 1.245
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.009 SNIP 1.3
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 0.985 SNIP 1.349
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 1.193 SNIP 1.301
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 0.722 SNIP 1.101
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 0.966 SNIP 1.284
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 0.87 SNIP 0.898
Web of Science (2000): Indexed yes
Scopus rating (1999): SJR 0.938 SNIP 0.885

Original language: English
Supercritical fluids, High pressure, Adsorption, Potential theory, Modeling
DOIs:
The Effects of Possible Contamination on the Radiocarbon Dating of the Dead Sea Scrolls II: Empirical Methods to Remove Castor Oil and Suggestions for Redating

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering, University of Southern Denmark
Authors: Rasmussen, K. L. (Ekstern), van der Plicht, J. (Ekstern), Doudna, G. (Ekstern), Nielsen, F. (Ekstern), Højrup, P. (Ekstern), Stenby, E. H. (Intern), Pedersen, C. T. (Ekstern)
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Web of Science (2018): Indexed yes
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BFI (2016): BFI-level 1
Scopus rating (2016): SJR 4.101 SNIP 2.736 CiteScore 4.53
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 3.425 SNIP 2.377 CiteScore 3.8
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.497 SNIP 1.464 CiteScore 1.97
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.808 SNIP 1.342 CiteScore 1.74
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 4.032 SNIP 2.679 CiteScore 3.93
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 3.14 SNIP 1.89 CiteScore 2.7
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.601 SNIP 1.877
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.878 SNIP 1.038
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.373 SNIP 0.459
Scopus rating (2007): SJR 3.167 SNIP 2.998
Scopus rating (2006): SJR 2.644 SNIP 1.909
Scopus rating (2005): SJR 0.534 SNIP 0.941
Scopus rating (2004): SJR 1.332 SNIP 2.135
Scopus rating (2003): SJR 0.515 SNIP 0.537
Scopus rating (2002): SJR 0.713 SNIP 0.672
Scopus rating (2001): SJR 3.612 SNIP 3.057
Thermodynamic Modeling of Several Aqueous Alkanol Solutions Containing Amino Acids with the Perturbed-Chain Statistical Associated Fluid Theory Equation of State

The perturbed-chain statistical associated fluid theory EoS was applied to model the solubilities of glycine, DL-alanine, L-serine, L-threonine, and L-isoleucine in pure water, pure alcohols (ethanol, 1-propanol, and 2-propanol) and in mixed solvent systems. Three pure component nonassociating parameters for the amino acids were fitted to the densities, activity and osmotic coefficients, vapor pressures, and water activity of their aqueous solutions. The solubilities of amino acids in pure and mixed solvent systems were calculated on the basis of the phase equilibrium conditions for a pure solid and a fluid phase. The hypothetical melting properties of each amino acid were fitted, to accurately correlate the solubilities in pure water. Only one temperature independent binary parameter is required for each amino acid/solvent pair. The model can accurately describe the solubility of the amino acids in water, but the correlation for the solubility in pure alcohols was not so satisfactory. The solubility in mixed solvents (ternary systems) was predicted on the basis of the modeling of the solubility in pure solvents, without any additional fitting of the parameters, and the results achieved were reasonable. Fitting the binary parameter for the pair amino acid/alcohol not to the solubility in pure alcohol, but to the solubility in the mixed solvent system, the description of the solubility in the mixed solvent systems was clearly improved and the results were in fair agreement with the experimental data for all mixture compositions. The results showed a global root-mean-square deviation in mole fraction of 0.0032 for correlation and 0.0070 for prediction.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Phase Equilibria and Separation Processes, Center for Energy Resources Engineering
Authors: Ferreira, L. (Intern), Breil, M. P. (Intern), Pinho, S. P. (Ekstern), Macedo, E. A. (Ekstern), Mollerup, J. (Intern)
Pages: 5498-5505
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Scopus rating (2016): CiteScore 3.1 SJR 0.945 SNIP 1.139
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.949 SNIP 1.146 CiteScore 2.87
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.012 SNIP 1.292 CiteScore 2.85
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 0.982 SNIP 1.243 CiteScore 2.6
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.066 SNIP 1.338 CiteScore 2.56
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
Thermodynamic Modeling of Water-Acid Gases-Alkanolamine Systems

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Sadegh, N. (Intern), Thomsen, K. (Intern), Stenby, E. H. (Intern), Kontogeorgis, G. (Intern)
Publication date: 2009

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ISBN (Print): 978-0-8169-1058-6
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 255352
Publication: Research - peer-review » Article in proceedings – Annual report year: 2009
Thermodynamics of Triethylene Glycol and Tetraethylene Glycol Containing Systems Described by the Cubic-Plus-Association Equation of State

A thorough investigation of triethylene glycol (TEG) containing systems has been performed. The introduction of a new six-site association scheme for the TEG molecule has shown to be advantageous. Glycols are often modeled using a four-site scheme (abbreviated as 4C) hence ignoring the internal lone pairs of oxygen. The new association scheme also takes these sites into account. The new parameters of TEG are based on the vapor pressure data, liquid density data, and liquid-liquid equilibria (LLE) data (n-heptane), and they are tested for binary systems (methane, n-octane, n-nonane, n-decane, benzene, toluene, ethylbenzene, and water) and different types of phase equilibria (vapor-liquid equilibria (VLE) and LLE) and thermodynamic properties (heat of mixing, activity coefficients). A less extensive investigation has also been performed on tetraethylene glycol (TeEG) containing systems. Similarly, a new seven-site association scheme for the TeEG molecule has been investigated. The new parameters of TeEG are based on vapor pressure data, liquid density data, and LLE data (n-heptane). The performance is similar to that of the 4C scheme.
A predictive group-contribution simplified PC-SAFT equation of state: Application to polymer systems

A group-contribution (GC) method is coupled with the molecular-based perturbed-chain statistical associating fluid theory (PC-SAFT) equation of state (EoS) to predict its characteristic pure compound parameters. The estimation of group contributions for the parameters is based on a parameter database of 400 low-molecular-weight compounds estimated by fitting experimental vapor pressures and liquid densities. The method has been successfully used for estimating the PC-SAFT parameters for common polymers. Specifically, using the new polymer parameters as calculated from the proposed GC scheme, the simplified PC-SAFT yields rather good predictions of polymer densities and gives promising modeling results of various binary polymer mixtures exhibiting both vapor-liquid and liquid-liquid phase equilibria. In summary, the data required for calculating polymer phase equilibria with the proposed method are the molecular structure of the polymer of interest in terms of functional groups and a single binary interaction parameter for accurate mixture calculations.

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
A review of the thermodynamics of protein association to ligands, protein adsorption, and adsorption isotherms

The application of thermodynamic models in the development of chromatographic separation processes is discussed. The paper analyses the thermodynamic principles of protein adsorption. It can be modeled either as a reversible association between the adsorbate and the ligands or as a steady-state process where the rate of adsorption is equal to the rate of desorption. The analysis includes the competitive Langmuir isotherm and the exponentially modified Langmuir isotherm. If the adsorbate binds to one ligand only, the different approaches become identical. When the adsorbate acts as a ligand, dimerization takes place and will give rise to a sigmoid isotherm. A model that accounts for dimerization is discussed and a sample calculation shows the behavior of this isotherm. Insulin is known to have a concave isotherm at low concentrations. The calculation of the standard Gibbs energy change of adsorption is discussed. Hydrophobic and reversed phase chromatography are useful techniques for measuring solute activity coefficients at infinite dilution.

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Mollerup, J. (Intern)
Pages: 864-874
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Ratings:
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Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 0.525 SNIP 0.872 CiteScore 1.47
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.613 SNIP 0.916 CiteScore 1.57
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.701 SNIP 0.999 CiteScore 1.68
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.724 SNIP 1.048 CiteScore 1.83
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Capture and Storage Projects at IVC-SEP

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Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Center for Energy Resources Engineering, CERE – Center for Energy Resources Engineering, Department of Chemistry
Publication date: 2008
Event: Poster session presented at DTU Energy Conference, Technical University of Denmark, Copenhagen, DK
Main Research Area: Technical/natural sciences
Electronic versions:
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Source: orbit
Source-ID: 232201
Publication: Research - peer-review › Poster – Annual report year: 2008

Chilled ammonia process for CO2 capture

General information
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Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Darde, V. C. A. (Intern), Thomsen, K. (Intern), Stenby, E. H. (Intern)
Publication date: 2008

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Elliptic random-walk equation for suspension and tracer transport in porous media

We propose a new approach to transport of the suspensions and tracers in porous media. The approach is based on a modified version of the continuous time random walk (CTRW) theory. In the framework of this theory we derive an elliptic transport equation. The new equation contains the time and the mixed dispersion terms expressing the dispersion of the particle time steps. The properties of the new equation are studied and the fundamental analytical solutions are obtained.

The solution of the pulse injection problem describing a common tracer injection experiment is studied in greater detail. The new theory predicts delay of the maximum of the tracer, compared to the velocity of the flow, while its forward "tail" contains much more particles than in the solution of the classical parabolic (advection-dispersion) equation. This is in agreement with the experimental observations and predictions of the CTRW theory. (C) 2008 Elsevier B.V. All rights reserved.
Evaluation of the nonrandom hydrogen bonding (NRHB) theory and the simplified perturbed-chain-statistical associating fluid theory (sPC-SAFT). 1. Vapor-liquid equilibria

A standard database for the validation of vapor-liquid equilibrium (VLE) models was used to evaluate prediction and correlation accuracy of the nonrandom hydrogen bonding (NRHB) theory and the simplified perturbed-chain-statistical associating fluid theory (PC-SAFT). Pure-component parameters for the models were taken from literature or estimated in this work. Generalized pure-component parameters were fitted to pure-component vapor-pressure and liquid-density data. For the majority of the mixtures examined, satisfactory results were obtained. For a number of mixtures, different modeling approaches were applied to improve the results, such as incorporation of cross-association between nonself-associating fluids or induced association for mixtures of polar nonassociating and self-associating fluids. For both models, the overall deviations from experimental data are similar, and none of the models is found to be overall superior over the other. However, for specific mixtures, one model often performs better than the other.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Phase Equilibria and Separation Processes, Center for Energy Resources Engineering
Authors: Grenner, A. (Intern), Tsivintzelis, I. (Intern), Economou, I. (Intern), Panayiotou, C. (Ekstern), Kontogeorgis, G. (Intern)
Pages: 5636-5650
Publication date: 2008
Main Research Area: Technical/natural sciences

Publication information
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Volume: 47
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BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.1 SJR 0.945 SNIP 1.139
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.949 SNIP 1.146 CiteScore 2.87
Two statistical thermodynamic models, the nonrandom hydrogen bonding (NRHB) theory, which is a compressible lattice model, and the simplified perturbed-chain-statistical associating fluid theory (sPC-SAFT), which is based on Wertheim's perturbation theory, were used to model liquid-liquid equilibria and predict the fraction of nonhydrogen bonded molecules in various hydrogen bonding mixtures. Carefully selected binary mixtures, which include water-hydrocarbon, 1-alkanol-hydrocarbon, water-1-alkanol, and glycol-hydrocarbon, were used to benchmark the accuracy of the models. Both models...
yielded satisfactory and often very similar results for the phase behavior of the investigated mixtures. sPC-SAFT yielded more accurate predictions, while NRHB yielded more accurate correlations, in mixtures of water with normal alkanes and cycloalkanes. In water-aromatic hydrocarbon mixtures, satisfactory correlations were obtained only when solvation was accounted for. Both models resulted in satisfactory correlations for all other mixtures, while for specific mixtures, one model may perform better than the other. Finally, both models, despite that they are based on totally different approaches for the treatment of hydrogen bonding, yielded similar predictions for the fraction of non-hydrogen bonded molecules (monomer fraction) in pure 1-alkanols and in 1-alkanol-n-hexane mixtures.
Gas transport in tight porous media Gas kinetic approach
We describe the flow of gas in a porous medium in the kinetic regime, where the viscous flow structure is not formed in separate pores. Special attention is paid to the dense kinetic regime, where the interactions within the gas are as important as the interaction with the porous medium. The transport law for this regime is derived by means of the gas kinetic theory, in the framework of the model of "heavy gas in light one". The computations of the gas kinetic theory are confirmed by the dimension analysis and a simplified derivation revealing the considerations behind the kinetic derivation. The role of the thermal gradient in the transport law is clarified. (c) 2007 Elsevier B.V. All rights reserved.
Modeling of biopharmaceutical processes. Part 2: Process chromatography unit operation

Process modeling can be a useful tool to aid in process development, process optimization, and process scale-up. When modeling a chromatography process, one must first select the appropriate models that describe the mass transfer and adsorption that occurs within the porous adsorbent. The theoretical understanding of chromatographic behavior can augment available experimental data and aid in the design of specific experiments to develop a more complete understanding of the behavior of a unit operation.

General information
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Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Kaltenbrunner, O. (Ekstern), McCue, J. (Ekstern), Engel, P. (Ekstern), Mollerup, J. (Intern), Rathore, A. S. (Ekstern)
Modeling systems containing alkanolamines with the CPA equation of state

An association model, the cubic-plus-association (CPA) equation of state (EoS), is applied for the first time to a class of multifunctional compounds (alkanolamines). Three alkanolamines of practical and scientific significance are considered; monoethanolamine (MEA), diethanolamine (DEA), and methyl diethanolamine (MDEA). Vapor pressures and liquid densities, as well as solvatochromic parameters and mixture liquid−liquid equilibria (LLE) data with alkanes are used to estimate the five pure-compound parameters. Vapor−liquid equilibria (VLE) calculations for cross-associating mixtures, especially those with water, are used in the validation of the parameters. The influence on the results of the association scheme, cross-association combining rules, interaction parameters, and the data available is discussed also, in
connection with other aqueous cross-associating mixtures previously studied using the CPA equation of state (alcohols, amines, and glycols).

**General information**

State: Published

Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering

Authors: Avlund, A. S. (Intern), Kontogeorgis, G. (Intern), Michelsen, M. L. (Intern)

Pages: 7441-7446

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Main Research Area: Technical/natural sciences

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Web of Science (2018): Indexed yes

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Web of Science (2017): Indexed yes

BFI (2016): BFI-level 2

Scopus rating (2016): CiteScore 3.1 SJR 0.945 SNIP 1.139

Web of Science (2016): Indexed yes

BFI (2015): BFI-level 2

Scopus rating (2015): SJR 0.949 SNIP 1.146 CiteScore 2.87

Web of Science (2015): Indexed yes

BFI (2014): BFI-level 2

Scopus rating (2014): SJR 1.012 SNIP 1.292 CiteScore 2.85

Web of Science (2014): Indexed yes

BFI (2013): BFI-level 2

Scopus rating (2013): SJR 0.982 SNIP 1.243 CiteScore 2.6

ISI indexed (2013): ISI indexed yes

Web of Science (2013): Indexed yes

BFI (2012): BFI-level 2

Scopus rating (2012): SJR 1.066 SNIP 1.338 CiteScore 2.56

ISI indexed (2012): ISI indexed yes

Web of Science (2012): Indexed yes

BFI (2011): BFI-level 2

Scopus rating (2011): SJR 1.086 SNIP 1.24 CiteScore 2.58

ISI indexed (2011): ISI indexed yes

Web of Science (2011): Indexed yes

BFI (2010): BFI-level 2

Scopus rating (2010): SJR 1.047 SNIP 1.165

Web of Science (2010): Indexed yes

BFI (2009): BFI-level 2

Scopus rating (2009): SJR 1.002 SNIP 1.164

Web of Science (2009): Indexed yes

BFI (2008): BFI-level 2

Scopus rating (2008): SJR 1.142 SNIP 1.267

Web of Science (2008): Indexed yes

Scopus rating (2007): SJR 1.105 SNIP 1.239

Web of Science (2007): Indexed yes

Scopus rating (2006): SJR 1.035 SNIP 1.204

Web of Science (2006): Indexed yes

Scopus rating (2005): SJR 0.993 SNIP 1.241
Modelling of phase equilibria of glycol ethers mixtures using an association model

Vapor-liquid and liquid-liquid equilibria of glycol ethers (surfactant) mixtures with hydrocarbons, polar compounds and water are calculated using an association model, the Cubic-Plus-Association Equation of State. Parameters are estimated for several non-ionic surfactants of the polyoxyethylene type but mixture calculations are mostly presented for three compounds for which many data are available (2-methoxyethanol, 2-ethoxyethanol and 2-butoxyethanol). The way pure compound vapor pressures and liquid densities are estimated, and the way parameter trends against the van der Waals volume, Kamlet-Taft parameters and, perhaps most importantly, mixture liquid-liquid equilibria data with alkanes are used for choosing optimum parameter sets is illustrated. Vapor-liquid, liquid-liquid equilibria and second virial coefficient data are used for model validation, including aqueous and other cross-associating mixtures. The influence on the results of the association schemes, type of data available, combining rules for cross-associating mixtures and interaction parameters are discussed also in connection to other cross-associating mixtures, previously studied with the model. Finally, the capabilities and limitations of the Cubic-Plus-Association Equation of State in representing this type of multi-functional chemicals, glycol ethers, are discussed. (C) 2008 Elsevier B.V. All rights reserved.
Multi-Scale Modeling of Structure, Dynamic and Thermodynamic Properties of Imidazolium-Based Ionic Liquids: Ab Initio DFT Calculations, Molecular Simulation and Equation of State Predictions

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Economou, I. (Intern), Karakatsani, E. K. (Ekstern), Logotheti, G. -. (Ekstern), Ramos, J. (Ekstern), Vanin, A. (Ekstern)

DOI: 10.1016/j.fluid.2008.08.006
Source: orbit
Source-ID: 235786
Publication: Research - peer-review › Journal article – Annual report year: 2008
Phase equilibrium modelling for mixtures with acetic acid using an association equation of state

Acetic acid is a very important compound in the chemical industry with applications both as solvent and intermediate in the production of, e.g., polyesters. The design of these processes requires knowledge of the phase equilibria of mixtures.
containing acetic acid and a wide variety of compounds over extended temperature and pressure ranges. From the scientific point of view, modeling of such equilibria is challenging because of the complex association and solvation phenomena present. In this work, a previously developed association equation of state (cubic-plus-association, CPA) is applied to a wide variety of mixtures containing acetic acid, including gas solubilities, cross-associating systems (with water and alcohols), and polar chemicals like acetone and esters. Vapor-liquid and liquid-liquid equilibria are considered for both binary and ternary mixtures. With the exception of a somewhat inferior performance for the water-acetic acid VLE, which does not seem to affect substantially the performance for the multicomponent systems studied, CPA performs satisfactorily in most cases, using a single interaction parameter over extensive temperature ranges. For accurate description of water-acetic acid, use of the Huron-Vidal mixing rule for the energy parameter of CPA can yield a satisfactory correlation at the cost of more interaction parameters.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Phase Equilibria and Separation Processes, Center for Energy Resources Engineering
Authors: Muro Sunè, N. (Intern), Kontogeorgis, G. (Intern), von Solms, N. (Intern), Michelsen, M. L. (Intern)
Pages: 5660-5668
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Main Research Area: Technical/natural sciences

Publication information
Journal: Industrial & Engineering Chemistry Research
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BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.1 SJR 0.945 SNIP 1.139
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.949 SNIP 1.146 CiteScore 2.87
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.012 SNIP 1.292 CiteScore 2.85
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 0.982 SNIP 1.243 CiteScore 2.6
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.066 SNIP 1.338 CiteScore 2.56
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.086 SNIP 1.24 CiteScore 2.58
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.047 SNIP 1.165
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.002 SNIP 1.164
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Propane hydrate nucleation: Experimental investigation and correlation

In this work the nucleation kinetics of propane gas hydrate has been investigated experimentally using a stirred batch reactor. The experiments have been performed isothermally recording the pressure as a function of time. Experiments were conducted at different stirring rates, but in the same supersaturation region. The experiments showed that the gas dissolution rate rather than the induction time of propane hydrate is influenced by a change in agitation. This was especially valid at high stirring rates when the water surface was severely disturbed. Addition of polyvinylpyrrolidone (PVP) to the aqueous phase was found to reduce the gas dissolution rate slightly. However, the induction times were prolonged quite substantially upon addition of PVP. The induction time data were correlated using a newly developed induction time model based on crystallization theory also capable of taking into account the presence of additives. In most cases reasonable agreement between the data and the model could be obtained. The results revealed that especially the effective surface energy between propane hydrate and water is likely to change when the stirring rate varies from very high to low. The prolongation of induction times according to the model is likely to be due to a change in the nuclei-substrate contact angle.

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Jensen, L. (Intern), Thomsen, K. (Intern), von Solms, N. (Intern)
Pages: 3069-3080
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Main Research Area: Technical/natural sciences

Publication information
Journal: Chemical Engineering Science
Volume: 63
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BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
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Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.05 SJR 1.037 SNIP 1.442
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.038 SNIP 1.606 CiteScore 2.96
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.115 SNIP 1.642 CiteScore 2.81
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.157 SNIP 1.866 CiteScore 2.95
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.189 SNIP 1.847 CiteScore 2.77
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.205 SNIP 1.685 CiteScore 2.8
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.319 SNIP 1.708
Web of Science (2010): Indexed yes
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Scopus rating (2009): SJR 1.293 SNIP 1.759
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 1.299 SNIP 1.6
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.347 SNIP 1.523
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.308 SNIP 1.553
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.445 SNIP 1.801
Scopus rating (2004): SJR 1.301 SNIP 1.858
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 1.7 SNIP 1.676
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 1.675 SNIP 1.279
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 1.706 SNIP 1.734
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 1.313 SNIP 1.307
Web of Science (2000): Indexed yes
Scopus rating (1999): SJR 1.214 SNIP 1.539
Original language: English
DOIs:
10.1016/j.ces.2008.03.006
Source: orbit
Source-ID: 204995
Publication: Research - peer-review › Journal article – Annual report year: 2008
Random-Walk Description of Suspension Transport in Porous Media

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Bedrikovetsky, P. (Ekstern), Shapiro, A. (Intern)
Publication date: 2008

Host publication information
Title of host publication: ICTAM 2008
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 219857
Publication: Research - peer-review › Article in proceedings – Annual report year: 2008

Solvation phenomena in association theories with applications to oil & gas and chemical industries

Association theories e.g. those belonging to the SAFT family account explicitly for self- and cross-association (solvation) phenomena. Such phenomena are of great practical importance as they affect, often dramatically, the phase behaviour of many mixtures of industrial relevance. From the scientific point of view, solvation phenomena are also very significant because they are present in different types of mixtures and not just those containing two self-associating compounds e.g. water with alcohols or glycols. Mixtures with only one self-associating compound and in some cases even mixtures with two non self-associating compounds may exhibit solvation specifically due to hydrogen bonding or more generally due to Lewis acid-Lewis base interactions. As examples can be mentioned mixtures with polar compounds (water, glycols...) and aromatic hydrocarbons and aqueous ether or ester solutions. This manuscript presents how a specific association thermodynamic model, which employs SAFT’s association term, the so-called CPA (Cubic-Plus-Association) equation of state, can be applied in order to account for various types of interactions due to solvation. The role of combining rules in the association term and the cases where explicit treatment of solvation is needed will be illustrated.

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Kontogeorgis, G. (Intern), Folas, G. (Intern), Muro Sunè, N. (Intern), Roca Leon, F. (Intern), Michelsen, M. L. (Intern)
Pages: 305-319
Publication date: 2008
Main Research Area: Technical/natural sciences

Publication information
Journal: Oil & Gas Science & Technology
Volume: 63
Issue number: 3
ISSN (Print): 1294-4475
The chilled ammonia process - Evaluation of the energy requirements

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Fosbøl, P. L. (Intern), Stenby, E. H. (Intern), Thomsen, K. (Intern)
Publication date: 2008

Publication information
Original language: English
The Influence of CO2 Solubility in Brine on CO2 Flooding Simulation

General information
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Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Yan, W. (Intern), Stenby, E. H. (Intern)
Publication date: 2008

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Title of host publication: 29th IEA Workshop and Symposium 2008
Main Research Area: Technical/natural sciences
Conference: IEA Workshop and Symposium Collaborative Project on Enhanced Oil Recovery, Beijing, China, 01/01/2008
Source: orbit
Source-ID: 236537
Publication: Research - peer-review › Article in proceedings – Annual report year: 2008

A Computational Efficient and Robust Implementation of the Continuous-Discrete Extended Kalman Filter

General information
State: Published
Organisations: Scientific Computing, Department of Informatics and Mathematical Modeling, Mathematical Statistics, Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Jørgensen, J. B. (Intern), Thomsen, P. G. (Intern), Madsen, H. (Intern), Kristensen, M. R. (Intern)
Publication date: 2007

Host publication information
Title of host publication: Proceeding of the American Control Conference
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 207459
Publication: Research - peer-review › Article in proceedings – Annual report year: 2007

Application of PC-SAFT to glycol containing systems - PC-SAFT towards a predictive approach
For equations of state of the SAFT type a major limitation is the procedure of obtaining pure compound parameters using saturated vapor pressure and liquid density data. However, for complex compounds such data are often not available. One solution is to develop a group contribution scheme for estimating pure compound parameters from low molecular weight data and extrapolate to complex compounds. For associating compounds this is not trivial since the two parameters for association (association energy and association volume) need to be fixed for a group. In this work, which focuses on glycols, new general pure compound parameters were obtained for PC-SAFT which are able to perform well for both vapor-liquid equilibria (VLE) and liquid-liquid equilibria (LLE). Linear trends of non-association parameters were obtained with respect to the molar mass. However, identical values for the association parameters were used for all glycol oligomers. This makes it possible to predict the pure compound parameters of other oligomers. With the new estimated parameters the simplified PC-SAFT equation of state has been applied for correlation and prediction of VLE and LLE in mixtures containing glycol oligomers +water, hydrocarbons, aromatic hydrocarbon, methane, N-2 and CO2. To improve correlations for mixtures containing glycol and aromatic hydrocarbons solvation was explicitly accounted for. (C) 2007 Elsevier B.V. All rights reserved.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Phase Equilibria and Separation Processes, Center for Energy Resources Engineering
Authors: Grenner, A. (Intern), Kontogeorgis, G. (Intern), von Solms, N. (Intern), Michelsen, M. L. (Intern)
Pages: 248-257
Publication date: 2007
A stochastic model for filtration of particulate suspensions with incomplete pore plugging

A population balance model for particulate suspension transport with capture of particles by porous medium accounting for complete and incomplete plugging of pores by retained particles is derived. The model accounts for pore space accessibility, due to restriction on finite size particle movement through the overall pore space, and for particle flux reduction, due to transport of particles by the fraction of the overall flux. The novel feature of the model is the residual pore conductivity after the particle retention in the pore and the possibility of one pore to capture several particles. A closed system of governing stochastic equations determines the evolution of size distributions for suspended particles and pores. Its averaging results in the closed system of hydrodynamic equations accounting for permeability and porosity reduction due to plugging. The problem of deep bed filtration of a single particle size suspension through a single pore size medium where a pore can be completely plugged by two particles allows for an exact analytical solution. The phenomenological deep bed filtration model follows from the analytical solution.
Automated calculation of complete Pxy and Txy diagrams for binary systems

An algorithm for the calculation of global phase equilibrium diagrams has been recently developed [M. Cismondi, M.L. Michelsen, Global phase equilibrium calculations: critical lines, critical end points and liquid-liquid-vapour equilibrium in binary mixtures, J. Supercrit. Fluids 39 (2007) 287-295]. It integrates the calculation of critical lines, liquid-liquid-vapour (LLV) lines and critical end points, and was implemented in the software program GPEC: global phase equilibrium calculations [M. Cismondi, D.N. Nunez, M.S. Zabaloy, E.A. Brignole, M.L. Michelsen, J.M. Mollerup, GPEC: a program for global phase equilibrium calculations in binary systems, in: Proceedings of the CD-ROM EQUIFASE 2006, Morelia, Michoacan, Mexico, October 21-25, 2006; www.gpec.plapiqui.edu.ar]. In this work we present the methods and computational strategy for the automated calculation of complete Pxy and Txy diagrams in binary systems. Being constructed from the points given by the global phase diagram at a specified temperature or pressure, their calculation does not require the implementation of stability analysis. We illustrate the application of the algorithm through a variety of Pxy and Txy diagrams generated using the RK-PR EOS.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Phase Equilibria and Separation Processes, Center for Energy Resources Engineering
Authors: Cismondi, M. (Intern), Michelsen, M. L. (Intern)
Pages: 228-234
Publication date: 2007
Main Research Area: Technical/natural sciences

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BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 2.33 SJR 0.869 SNIP 1.155
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.874 SNIP 0.998 CiteScore 1.99
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 0.982 SNIP 1.248 CiteScore 2.28
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.007 SNIP 1.274 CiteScore 2.31
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.152 SNIP 1.286 CiteScore 2.31
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.034 SNIP 1.234 CiteScore 2.26
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 0.986 SNIP 1.317
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.133 SNIP 1.164
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.227 SNIP 1.09
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.031 SNIP 1.151
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.034 SNIP 1.245
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.009 SNIP 1.3
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 0.985 SNIP 1.349
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 1.193 SNIP 1.301
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 0.722 SNIP 1.101
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 0.966 SNIP 1.284
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 0.87 SNIP 0.898
Web of Science (2000): Indexed yes
Scopus rating (1999): SJR 0.938 SNIP 0.885

Original language: English
Pxy, calculation, Txy, phase diagrams, equations of state, binary systems
DOIs:
Calculation of the effect of macromolecular architecture on structure and thermodynamic properties of linear-tri-arm polyethylene blends from Monte Carlo simulation

A Monte Carlo simulation formalism proposed recently [Peristeras et al. Macromolecules 2007;40:2904-14] is applied here to linear-tri-arm polyethylene blends using atomistic models. Elementary Monte Carlo moves for long chain and branched molecules are used and shown to result in efficient relaxation of long chains. The effect of chain and arm molecular weight and of temperature on the structure and thermodynamic properties of blends is examined. Chemical potential versus composition diagrams are drawn in order to assess the non-ideality of mixing that may lead to phase separation. All of the blends examined are shown to be fully miscible. The microscopic blend structure is examined by calculating the radial distribution function. Finally, the radii of gyration of linear and branched chains are calculated and scaling exponents are evaluated.

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Rissanou, A. N. (Ekstern), Peristeras, L. D. (Ekstern), Economou, I. (Intern)
Pages: 3883-3892
Publication date: 2007
Main Research Area: Technical/natural sciences

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Journal: Polymer
Volume: 48
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Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.77 SJR 1.191 SNIP 1.252
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.157 SNIP 1.286 CiteScore 3.72
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.321 SNIP 1.619 CiteScore 3.85
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.415 SNIP 1.666 CiteScore 4.07
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.591 SNIP 1.8 CiteScore 3.74
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.623 SNIP 1.82 CiteScore 4.04
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.851 SNIP 1.8
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.999 SNIP 1.72
Calculation of the interfacial tension of the methane-water system with the linear gradient theory
The linear gradient theory (LGT) combined with the Soave-Redlich-Kwong (SRK EoS) and the Peng-Robinson (PR EoS) equations of state has been used to correlate the interfacial tension data of the methane-water system. The pure component influence parameters and the binary interaction coefficient for the mixture influence parameter have been obtained for this system. The model was successfully applied to correlate the interfacial tension data set to within 2.3% for the linear gradient theory and the SRK EoS (LGT-SRK) and 2.5% for the linear gradient theory and PR EoS (LGT-PR). A posteriori comparison of data not used in the parameterisation were to within 3.2% for the LGT-SRK model and 2.7% for the LGT-PR model. An exhaustive literature review resulted in a large database for the investigation which covers a wide range of temperature and pressures. The results support the success of the linear gradient theory modelling approach for this system. (C) 2007 Elsevier B.V. All rights reserved.
In this work, two "classical" (UNIFAC-FV, Entropic-FV) and two "recent" free-volume (FV) models (Kannan-FV, Freed-FV) are comparatively evaluated for polymer-solvent vapor-liquid equilibria including both aqueous and non-aqueous solutions. Moreover, some further developments are presented here to improve the performance of a recent model, the so-called Freed-FV. First, we propose a modification of the Freed-FV model accounting for the anomalous free-volume behavior of aqueous systems (unlike the other solvents, water has a lower free-volume percentage than polymers). The results predicted by the modified Freed-FV model for athermal and non-athermal polymer systems are compared to other "recent" and "classical" FV models, indicating an improvement for the modified Freed-FV model for aqueous polymer solutions. Second, for the original Freed-FV model, new UNIFAC group energy parameters are regressed for aqueous and alcohol solutions, based on the physical values of the van der Waals volume and surface areas for both FV-combinatorial and residual contributions. The prediction results of both "recent" and "classical" FV models using the new regressed energy parameters are significantly better, compared to using the classical UNIFAC parameters, for VLE of aqueous and alcohol polymer systems.
CO2 capture and storage

General information
State: Published
Organisations: UNEP Risoe Centre on Energy, Climate and Sustainable Development (URC), Systems Analysis Division, Risø National Laboratory for Sustainable Energy, Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Garg, A. (Intern), Appelquist, L. R. (Intern), Stenby, E. H. (Intern)
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Publisher: Danmarks Tekniske Universitet, Risø Nationallaboratoriumet for Bæredygtig Energi
Editors: Larsen, H. H., Sønderberg Petersen, L.
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Series: Denmark. Forskningscenter Risoe. Risoe-R
Number: 1612(EN)
ISSN: 0106-2840
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Electronic versions:
ris_r_1612.pdf
Source: orbit
Source-ID: 207112
Publication: Research - peer-review › Book chapter – Annual report year: 2007
Corrigendum to "High-pressure viscosity behavior of x 1,1,1,2-tetrafluoroethane (HFC-134a) + (1 - x) triethylene glycol dimethylether (TriEGDME) mixtures: Measurements and modeling" [Fluid Phase Equilibria, 247 (2006) 70-79]

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Monsalvo, M. A. (Intern), Baylauq, A. (Ekstern), Quiñones-Cisneros, S. E. (Ekstern), Boned, C. (Ekstern)
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Main Research Area: Technical/natural sciences

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Web of Science (2017): Indexed yes
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Scopus rating (2016): CiteScore 2.33 SJR 0.869 SNIP 1.155
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.874 SNIP 0.998 CiteScore 1.99
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 0.982 SNIP 1.248 CiteScore 2.28
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.007 SNIP 1.274 CiteScore 2.31
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.152 SNIP 1.286 CiteScore 2.31
Coupling Chemical Kinetics and Flashes in Reactive, Thermal and Compositional Reservoir Simulation

Phase changes are known to cause convergence problems for integration of stiff kinetics in thermal and compositional reservoir simulations. We propose an algorithm for detection and location of phase changes based on discrete event system theory. The algorithm provides a robust way for handling the switching of variables and equations required when the number of phases changes. We extend the method to handle full phase equilibrium described by an equation of state. Experiments show that the new algorithm improves the robustness of the integration process near phase boundaries by lowering the number of convergence and error test failures by more than 50% compared to direct integration without the new algorithm. To facilitate the algorithmic development we construct a virtual kinetic cell model. We use implicit one-step ESDIRK (Explicit Singly Diagonal Implicit Runge-Kutta) methods for integration of the kinetics. The kinetic cell model serves both as a tool for the development and testing of tailored solvers as well as a testbed for studying the interactions between chemical kinetics and phase behavior. A comparison between a K-value correlation based approach and a more rigorous equation of state based approach to phase equilibrium shows that phase behavior may significantly impact the reaction paths.
New data for the equilibrium water content of nitrogen, methane and one natural gas mixture are presented. The new binary data and existing binary sets were compared to calculated values of dew point temperature using both the CPA (Cubic-Plus-Association) EoS and the GERG-water EoS. CPA is purely predictive (i.e. all binary interaction parameters are set equal to 0), while GERG-water uses a temperature dependent interaction parameter fitted to published data. The GERG-water model is proposed as an ISO standard for determining the water content of natural gas. The data sets for nitrogen cover the range 233-348 K, and 5-200 bar. Six of these sets, including this work, are well described by both models; five of them have an average dew point temperature deviation of less than 1 K. The seventh set must be rejected, since the data points are too far removed from the other sets. The 13 sets for methane cover the range 233-373 K and 5-249 bar. Seven of these sets have an average bias less than 1 K, while another five have an average deviation less than 2 K. One set must be again rejected, having data too far from the other sets. Two of the remaining sets should probably be rejected as well, since they have large scatter. The data sets that have been measured at low pressures extrapolate well towards the ideal equilibrium values. The two models show similar results, but differ at high pressure and/or temperature. CPA is shown to extrapolate well for methane-water to 1000 bar and 573 K, and our conclusion is that GERG-water must be used with caution outside its specified working range. For some selected natural gas mixtures the two models also perform very much alike. The water content of the mixtures decreases with increasing amount of heavier components, and it seems that both models slightly over-predict the water content of such mixtures.
Development, modelling, optimisation and scale-up of chromatographic purification of a therapeutic protein

Development of a chromatographic purification step proceeds through a number of stages. High-throughput screening techniques are used to identify suitable resins. This technique is also suitable for the design of a capture step and some intermediate chromatographic steps, but development and true optimisation of a purification step necessitate simulations and thus models of the adsorption isotherm. A model for ion-exchange is reviewed and the strategy for estimation of model parameters is reported. Examples are shown where computer simulations are used for development and optimisation of chromatographic separations. Application of simulation of chromatographic processes supports innovation, efficiency and thus quality by design in biopharmaceutical development, manufacturing, and quality assurance and it enhances process understanding to facilitate innovation and risk-based regulatory decisions by industry. The theory of residence time based scale-up is developed and applied. (c) 2007 Elsevier B.V. All rights reserved.
Diffusion measurements in binary liquid mixtures by Raman spectroscopy

It is shown that Raman spectroscopy allows determination of the molar fractions in mixtures subjected to molecular diffusion. Spectra of three binary systems, benzene/n-hexane, benzene/cyclohexane, and benzene/acetone, were obtained during vertical (exchange) diffusion at several different heights (z) as a function of time. A procedure to determine time-dependent concentration profiles and diffusion coefficients is described in detail for one system, and results are given for the other two cases. For the system benzene/cyclohexane, much lower diffusion coefficients than reported in the literature were found, even in a thermostatically controlled diffusion cell, recording spectra through circulating water. For the system benzene/acetone, the determined diffusion coefficients were in good agreement with the literature data. The limitations of the Raman method are discussed, and it is concluded that many more systems ought to be studied. It is pointed out that diffusion profiles can be obtained in ternary and higher systems, where proper measurements are almost nonexistent.

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Efficient integration of stiff kinetics with phase change detection for reactive reservoir processes

We propose the use of implicit one-step Explicit Singly Diagonal Implicit Runge-Kutta (ESDIRK) methods for integration of the stiff kinetics in reactive, compositional and thermal processes that are solved using operator-splitting type approaches. To facilitate the algorithmic development we construct a virtual kinetic cell model. The model serves both as a tool for the development and testing of tailored solvers as well as a testbed for studying the interactions between chemical kinetics and phase behavior. As case study, two chemical kinetics models with 6 and 14 components, respectively, are implemented for in situ combustion, a thermal oil recovery process. Through benchmark studies using the 14 component reaction model the new ESDIRK solvers are shown to improve computational speed when compared to the widely used multi-step BDF methods DASSL and LSODE. Phase changes are known to cause convergence problems for the integration method. We propose an algorithm for detection and location of phase changes based on discrete event system theory. Experiments show that the algorithm improves the robustness of the integration process near phase boundaries by lowering the number convergence and error test failures by more than 50% compared to direct integration without the new algorithm.

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Elliptic equation for random walks. Application to transport in microporous media

We consider a process of random walks with arbitrary residence time distribution. We show that in many cases this process may not be described by the classical (Fick) parabolic diffusion equation, but an elliptic equation. An additional term proportional to the second time derivative takes into account the distribution of the residence times of molecules in pores. The new elliptic diffusion equation is strictly derived by the operator approach. A criterion showing where the new equation should be applied instead of the standard diffusion equation is obtained. Boundary conditions are studied and a principle for selection of a unique bounded solution is formulated. Fundamental solutions are obtained and compared with the results of direct simulation of the random walks. (c) 2006 Elsevier B.V. All rights reserved.
Equilibria in the mixed solvent system Glycol-NaOH-CO₂-Water applied to corrosion modelling

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Experimental investigation of liquid chromatography columns by means of computed tomography

The efficiency of packed chromatographic columns was investigated experimentally by means of computed tomography (CT) techniques. The measurements were carried out by monitoring tracer fronts in situ inside the chromatographic columns. The experimental results were fitted using the equilibrium dispersive model (EDM) and varying the so called apparent axial dispersion coefficient. The additivity of the first and second central moments was exploited to estimate column efficiency in different regions of the column. The results showed that the columns under investigation offered a higher column efficiency in the centre compared to the wall region. Furthermore the void fraction in the vicinity of the walls was lower than that in the column core. For this reason the bands were conveyed faster in the central region of the column where the permeability was higher. This result is in good agreement with earlier findings.

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Experimental validation of a rate-based model for CO2 capture using an AMP solution

Detailed experimental data, including temperature profiles over the absorber, for a carbon dioxide (CO₂) absorber with structured packing in an integrated laboratory pilot plant using an aqueous 2-amino-2-methyl-1-propanol (AMP) solution are presented. The experimental gas-liquid material balance was within an average of 3.5% for the experimental conditions presented. A predictive rate-based steady-state model for CO₂ absorption into an AMP solution, using an implicit expression for the enhancement factor, has been validated against the presented pilot plant data. Furthermore, a parameter sensitivity analysis for the proposed model has been carried out.
Fluid characterization for miscible EOR projects and CO2 sequestration

Accurate performance prediction of miscible enhanced-oil-recovery (EOR) projects or CO2 sequestration in depleted oil and gas reservoirs relies in part on the ability of an equation-of-state (EOS) model to adequately represent the properties of a wide range of mixtures of the resident fluid and the injected fluid(s). The mixtures that form when gas displaces oil in a porous medium will, in many cases, differ significantly from compositions created in swelling tests and other standard pressure/volume/temperature (PVT) experiments. Multicontact experiments (e.g., slimtube displacements) are often used to condition an EOS model before application in performance evaluation of miscible displacements. However, no clear understanding exists of the impact on the resultant accuracy of the selected characterization procedure when the fluid description is subsequently included in reservoir simulation. In this paper, we present a detailed analysis of the quality of two different characterization procedures over a broad range of reservoir fluids (13 samples) for which experimental swelling-test and slimtube-displacement data are available. We explore the impact of including swelling-test and slimtube experiments in the data reduction and demonstrate that for some gas/oil systems, swelling tests do not contribute to a more accurate prediction of multicontact miscibility. Finally, we report on the impact that use of EOS models based on different characterization procedures can have on recovery predictions from dynamic ID displacement calculations.

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Global phase equilibrium calculations: Critical lines, critical end points and liquid-liquid-vapour equilibrium in binary mixtures

A general strategy for global phase equilibrium calculations (GPEC) in binary mixtures is presented in this work along with specific methods for calculation of the different parts involved. A Newton procedure using composition, temperature and Volume as independent variables is used for calculation of critical lines. Each calculated point is analysed for stability by means of the tangent plane distance, and the occurrence of an unstable point is used to determine a critical endpoint (CEP). The critical endpoint, in turn, is used as the starting point for constructing the three-phase line. The equations for the critical endpoint, as well as for points on the three-phase line, are also solved using Newton's method with temperature, molar volume and composition as the independent variables. The different calculations are integrated into a general procedure that allows us to automatically trace critical lines, critical endpoints and three-phase lines for binary mixtures with phase diagrams of types from I to V without advance knowledge of the type of phase diagram. The procedure requires a thermodynamic model in the form of a pressure-explicit EOS but is not specific to a particular equation of state. (C) 2006 Elsevier B.V. All rights reserved.
High-pressure vapor-liquid equilibria of systems containing ethylene glycol, water and methane - Experimental measurements and modeling

This work presents new experimental phase equilibrium measurements of the binary MEG-methane and the ternary MEG-water-methane system at low temperatures and high pressures which are of interest to applications related to natural gas.
processing. Emphasis is given to MEG and water solubility measurements in the gas phase. The CPA and SRK EoS, the latter using either conventional or EoS/G(E) mixing rules are used to predict the solubility of the heavy components in the gas phase. It is concluded that CPA and SRK using the Huron-Vidal mixing rule perform equally satisfactory, while CPA requires fewer interaction parameters. (c) 2006 Elsevier B.V. All rights reserved.
Hybridization of the probability perturbation method with gradient information

Geostatistically based history-matching methods make it possible to devise history-matching strategies that will honor geologic knowledge about the reservoir. However, the performance of these methods is known to be impeded by slow convergence rates resulting from the stochastic nature of the algorithm. It is the purpose of this paper to introduce a method that integrates qualitative gradient information into the probability perturbation method to improve convergence. The potential of the proposed method is demonstrated on a synthetic history-matching example. The results indicate that inclusion of qualitative gradient information improves the performance of the probability perturbation method.

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In this work, the influence of structured packing on gas holdup in gas-liquid-solid dispersions has been studied. The experiments were carried out in an empty column and in column containing structured packing operating under identical conditions. Glass beads and silicon carbide particles were used as the solid material and the volumetric fraction of solids was varied from 0% to around 10%. The liquid viscosity was strongly modified using water, CMC solution and glycerol. The experimental results obtained with both columns were compared with previous results obtained in two-phase bubble columns. The influence of structured packing on the total gas holdup for different superficial gas velocities was found to be similar with and without suspended solids. Therefore, the results obtained in this work were analysed on the basis of correlations derived earlier for gas-liquid dispersions. Excepting the results obtained with glycerol, these correlations can predict the gas holdup of three-phase bubble columns with reasonable accuracy. (C) 2007 Elsevier Ltd. All rights reserved.

Influence of structured packing on gas holdup in a three-phase bubble column

In this work, the influence of structured packing on gas holdup in gas-liquid-solid dispersions has been studied. The experiments were carried out in an empty column and in column containing structured packing operating under identical conditions. Glass beads and silicon carbide particles were used as the solid material and the volumetric fraction of solids was varied from 0% to around 10%. The liquid viscosity was strongly modified using water, CMC solution and glycerol. The experimental results obtained with both columns were compared with previous results obtained in two-phase bubble columns. The influence of structured packing on the total gas holdup for different superficial gas velocities was found to be similar with and without suspended solids. Therefore, the results obtained in this work were analysed on the basis of correlations derived earlier for gas-liquid dispersions. Excepting the results obtained with glycerol, these correlations can predict the gas holdup of three-phase bubble columns with reasonable accuracy. (C) 2007 Elsevier Ltd. All rights reserved.
Measurement and modelling of hydrogen bonding in 1-alkanol plus n-alkane binary mixtures

Two equations of state (simplified PC-SAFT and CPA) are used to predict the monomer fraction of 1-alkanols in binary mixtures with n-alkanes. It is found that the choice of parameters and association schemes significantly affects the ability of a model to predict hydrogen bonding in mixtures, even though pure-component liquid densities and vapour pressures are predicted equally accurately for the associating compound. As was the case in the study of pure components, there exists some confusion in the literature about the correct interpretation and comparison of experimental data and theoretical studies, which is clarified in the present work. New hydrogen bonding data based on infrared spectroscopy are reported for seven binary mixtures of alcohols and alkanes. (C) 2007 Elsevier B.V. All rights reserved.
Modeling adsorption of binary and ternary mixtures on microporous media

The goal of this work is to analyze the adsorption of binary and ternary mixtures on the basis of the multicomponent potential theory of adsorption (MPTA). In the MPTA, the adsorbate is considered as a segregated mixture in the external potential field emitted by the solid adsorbent. This makes it possible using the same equation of state to describe the thermodynamic properties of the segregated and the bulk phases. For comparison, we also used the ideal adsorbed solution theory (IAST) to describe adsorption equilibria. The main advantage of these two models is their capabilities to predict multicomponent adsorption equilibria on the basis of single-component adsorption data. We compare the MPTA and IAST models to a large set of experimental data, obtaining reasonable good agreement with experimental data and high degree of predictability. Some limitations of both models are also discussed.
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Scopus rating (2009): SJR 1.133 SNIP 1.164
Web of Science (2009): Indexed yes
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Scopus rating (2008): SJR 1.227 SNIP 1.09
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Modeling phase equilibria of alkanols with the simplified PC-SAFT equation of state and generalized pure compound parameters

The simplified PC-SAFT equation of state has been applied to liquid-liquid, vapor-liquid and solid-liquid equilibria for mixtures containing 1-or 2-alkanols with alkanes, aromatic hydrocarbons, CO2 and water. For the alkanols we use generalized pure compound parameters. This means that two of the physical pure compound parameters, in (segment number) and or (segment diameter), are obtained from linear extrapolations, since m and m sigma(3), increase linearly with respect to the molar mass, and moreover, the two association parameters (association energy and association volume) were assumed to be constant for all alkanols. Only the dispersion energy is fitted to experimental data. Thus it is possible to estimate parameters for several 1-and 2-alkanols. The final aim is to develop a group contribution approach for PC-SAFT which is suitable for complex compounds, considering that the motivation of this project is to obtain a thermodynamic model which can be used in the development of sophisticated products such as pharmaceuticals, polymers, detergents or food ingredients. One of the severe limitations in applying SAFT-type equations of state to these compounds is that the procedure for obtaining the pure compound parameters is usually based on fitting to saturated vapor pressure and liquid density data over an extended temperature range. However, such data are rarely available for complex compounds. To verify the new pure compound parameters, comparisons to ordinary optimized alkanol parameters, where all five pure compound parameters were fitted to experimental liquid density and vapor pressure data, were made. The results show that the new generalized alkanol parameters from this work perform at least as well as other alkanol parameter sets. (c) 2007 Elsevier B.V. All rights reserved.
Fluorocarbons (FCs) are a family of chemicals that are composed primarily of carbon and fluorine. They present weak intermolecular and strong intramolecular interactions, which confers them unusual thermophysical properties. They can also solubilize large amounts of gases such as oxygen and carbon dioxide, making them interesting for several biomedical applications. In most of these applications, water or aqueous systems are present for which the knowledge of the mutual solubilities between the fluorocarbons and the aqueous phases is important. In this work, the application of the cubic-plus-association equation of state (CPA EoS) has been extended to binary mixtures of water with several linear, cyclic, aromatic, and substituted fluorocarbons. The CPA EoS was successfully used to model the liquid-liquid equilibria of aqueous mixtures that contain FCs, while also being able to describe the cross-association phenomena between substituted and aromatic FCs and water. It is shown that, for aliphatic perfluorocarbons, CPA can be used without any mixture binary parameter to predict the water solubility.
Modelling of associating mixtures for applications in the oil & gas and chemical industries
Thermodynamic properties and phase equilibria of associating mixtures cannot often be satisfactorily modelled using conventional models such as cubic equations of state. CPA (cubic-plus-association) is an equation of state (EoS), which combines the SRK EoS with the association term of SAFT. For non-polar (non self-associating) compounds it reduces to SRK. The model was first published in 1996 and since then it has been developed and applied with success to binary systems containing water-alkanes and alcohol/glycol/acid-alkanes (both VLE and LLE) as well as ternary and multicomponent (V)LLE for water-alcohol (glycol)-alkanes and certain acid and amine-containing mixtures. Recent results include glycol-aromatic hydrocarbons including multiphase, multicomponent equilibria and gas hydrate calculations in combination with the van der Waals-Platteeuw model. This article will outline some new applications of the model of relevance to the petroleum and chemical industries: high pressure vapor-liquid and liquid-liquid equilibrium in alcohol-containing mixtures, mixtures with gas hydrate inhibitors and mixtures with polar and hydrogen bonding chemicals including organic acids. Some comparisons with conventional thermodynamic models especially those combining cubic EoS with local composition activity coefficient models are included. (C) 2007 Elsevier B.V. All rights reserved.
Multicomponent equations of state for electrolytes

Four equations of state have been implemented and evaluated for multicomponent electrolyte solutions at 298.15 K and 1 bar. The equations contain terms accounting for short-range and long-range interactions in electrolyte solutions. Short-range interactions are described by one of the three equations of state, Peng-Robinson, Soave-Redlich-Kwong, or Cubic-Plus-Association (CPA). Long-range interactions are described by either the simplified mean spherical approximation (MSA) solution of the Ornstein-Zernicke equation or the simplified Debye-Hückel term. An optional Born term is added to these electrostatic terms. The resulting electrolyte equations of state were tested by determining the optimal model parameters for the multicomponent test system consisting of H2O, Na+, H+, Ca2+, Cl-, OH-, SO42-. To describe the thermodynamics of this multicomponent system, ion specific parameters were determined. The parameters in the equations of state were fitted to experimental data consisting of apparent molar volumes, osmotic coefficients, mean ionic activity coefficients, and solid-liquid equilibrium data. The results of the parameter fitting are presented. The ability of the equations of state to reproduce the experimental data is demonstrated. The performance of the equations of state for multi component systems is compared and analyzed in view of the various short-range and long-range terms employed. (c) 2007 American Institute of Chemical Engineers.

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On the estimation of water pure compound parameters in association theories

Determination of the appropriate number of association sites and estimation of parameters for association (SAFT-type) theories is not a trivial matter. Building further on a recently published manuscript by Clark et al., this work investigates aspects of the parameter estimation for water using two different association theories. Their performance for various properties as well as against the results presented earlier is demonstrated.
Despite its industrial importance, adsorption from the liquid phase has been studied much less extensively than adsorption from the gas phase. In this paper, we study the adsorption of liquid mixtures on the basis of the multicomponent potential theory of adsorption (MPTA). The MPTA is based on the potential concept originally developed by Polanyi. In this theory, the driving force for physical adsorption is measured by the adsorption potential that is a function of the distance from the solid surface. In this way, the adsorbate is considered as a heterogeneous substance segregated in the external field emitted by the adsorbent, with thermodynamic parameters that are function of the distance from the solid. The MPTA then uses a thermodynamic model to describe the equilibrium between bulk and adsorbed phases (or the fluid-fluid interactions), and potential models for the fluid-solid interactions. With this approach, few parameters are needed to predict adsorption equilibria. The MPTA has been so far used to successfully predict adsorption equilibria of multicomponent gas mixtures. The aim of this work is to extend the MPTA onto adsorption from liquid solutions. We show that such extension is straightforward, obtaining relatively simple models useful for engineering applications. Comparison with experimental data shows good agreement and high degree of predictability. (C) 2007 Elsevier B.V. All rights reserved.
Predictions of flavonoid solubility in ionic liquids by COSMO-RS: experimental verification, structural elucidation, and solvation characterization

Predictions of the solubility of flavonoids in a large variety of ionic liquids (ILs) with over 1800 available structures were examined based on COSMO-RS computation. The results show that the solubilities of flavonoids are strongly anion-dependent. Experimental measurement of the solubilities of esculin and rutin in 12 ILs with varying anions and cations show that predicted and experimental results generally have a good agreement. Based on the sound physical basis of COSMO-RS, the solubility changes of flavonoids were quantitatively associated with solvation interactions and structural characteristics of ILs. COSMO-RS derived parameters, i.e. misfit, H-bonding and van der Waals interaction energy, are shown to be capable of characterizing the complicated multiple interactions in the IL system effectively. H-bonding interaction is the most dominant interaction for ILs (followed by misfit and van der Waals interactions) to determine the solubility of flavonoids, and the anionic part has greater effect on the overall H-bonding capability of the IL. Based on basicity of anions, ILs were categorized into 3 groups, corresponding to the classification of the solubility of flavonoid. COSMO sigma-moment descriptors, which roughly denote the characteristic properties of the ILs, might be of general value to have a fast estimation for the solubilities of flavonoids as well as those compounds with massive moieties as H-bonding donors. The results obtained in this work may be important for achieving an improved understanding of IL solvations and the tailoring of the desired structures of ILs used as the media for efficient enzymatic esterification of flavonoids.
The solubility of n-alkanes, perfluoroalkanes, noble gases and light gases in four elastomer polymers containing silicon is examined based on molecular simulation and macroscopic equation of state modelling. Polymer melt samples generated from molecular dynamics (MD) are used for the calculation of gas and solvent solubilities using the test particle insertion method of Widom. Polymer chains are modelled using recently developed realistic atomistic force fields. Calculations are performed at various temperatures and ambient pressure. A crossover in the temperature dependence of solubility as a function of the gas/solvent critical temperature is observed for all polymers. A macroscopic model based on the simplified perturbed chain-statistical associating fluid theory (sPC-SAFT) is used for the prediction and correlation of solubilities in poly(dimethylsiloxane) and poly(dimethylsiloxane) and also the phase equilibria of these mixtures over a wide composition range. In all cases, the agreement between model predictions/correlations and literature experimental data, when available, is excellent.
Study of asphaltene precipitation by Calorimetry

Can calorimetry bring new input to the current understanding of asphaltene precipitation? In this work, two types of precipitation were studied by means of calorimetry: addition of n-heptane into asphaltene solutions and temperature/pressure variations on a recombined live oil. The first series of experiments showed that weak forces determine precipitation. Indeed, isothermal titration calorimetry could not detect any clear signal although this technique can detect low-energy transitions such as liquid-liquid equilibrium and micellization. The second series of tests proved that precipitation caused by T and P variations is exothermic for this system. Furthermore, the temperature-induced precipitation is accompanied by an increase in the apparent thermal expansivity. Therefore, it seems that these two phase transitions exhibit different calorimetric behaviours and they may not be as similar as expected.

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Organisations: Department of Chemical and Biochemical Engineering, Center for Phase Equilibria and Separation Processes, Center for Energy Resources Engineering
Study of the solubility of a modified Bacillus licheniformis alpha-amylase around the isoelectric point

The solubility of a modified recombinant Bacillus licheniformis alpha-amylase (mBLA) has been studied by batch crystallization. A semi-pure preparation was chosen containing five isoforms with pI values from 6 to 7.3 (weighted average of 6.6). Small amounts (<1 %) of protein impurities were also present. Solubility was studied in the pH range of 6 to 8. The lowest solubility without added salts was 60 mg.mL(-1) at pH 7. The addition of 0.1 mol.L-1 sodium salts of nitrate, sulfate, and thiocyanate had a small effect on solubility. However, solubility was lowered significantly by adding 0.5 mol.L-1 sodium sulfate at all pH values and increased with 0.5 mol.L-1 sodium thiocyanate at pH 7 and pH 8. The effect of anions on alpha-amylase solubility followed the Hofmeister series, and only weak evidence of reversal was seen below the isoelectric point. Cations had little effect on solubility. The sign and magnitude of the alpha-amylase zeta potential was determined in the presence and absence of 0.1 mol.L-1 salt. Qualitatively, zeta potential correctly predicted the different salts influence on mBLA solubility.
The Hansen Solubility Parameters (HSP) in Thermodynamic Models for Polymer Solutions

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Kontogeorgis, G. (Intern)
Number of pages: 75
Publication date: 2007

Host publication information
Title of host publication: Hansen Solubility Parameters - A user’s handbook by Charles Hansen
Publisher: C R C Press LLC
Edition: 2
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 199158
Publication: Research - peer-review › Book chapter – Annual report year: 2007

The influence of salt type on the retention of bovine serum albumin in ion-exchange chromatography
In this paper, an analysis of the influence of the salt types, NaCl, NaCH\textsubscript{3}COO, Na\textsubscript{2}SO\textsubscript{4} and Na\textsubscript{3}C\textsubscript{6}H\textsubscript{5}O\textsubscript{7}, on the isocratic retention behaviour of bovine serum albumin (BSA) on two anion-exchangers media (Source 30Q and TSK Gel Super Q 5 PW) has been presented. The retention data demonstrated that the mechanism of protein retention in ion-exchange chromatography (IEC) involves interactions between the protein solute, the mobile phase constituents and the stationary phase. The effect of protein activity coefficient in the mobile phase on the protein retention volumes is verified.

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Al-Jibbouri, S. (Intern)
Pages: 57-62
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- BFI (2018): BFI-level 1
- Web of Science (2018): Indexed yes
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- Web of Science (2017): Indexed Yes
- BFI (2016): BFI-level 1
- Scopus rating (2016): CiteScore 3.97 SJR 1.462 SNIP 1.295
- BFI (2015): BFI-level 1
- Scopus rating (2015): SJR 1.713 SNIP 1.395 CiteScore 4.03
- Web of Science (2015): Indexed yes
- BFI (2014): BFI-level 1
- Scopus rating (2014): SJR 1.825 SNIP 1.509 CiteScore 4.28
- Web of Science (2014): Indexed yes
- BFI (2013): BFI-level 1
- Scopus rating (2013): SJR 2.017 SNIP 1.616 CiteScore 4.6
- ISI indexed (2013): ISI indexed yes
- Web of Science (2013): Indexed yes
- BFI (2012): BFI-level 1
- Scopus rating (2012): SJR 2.31 SNIP 1.703 CiteScore 4.6
- ISI indexed (2012): ISI indexed yes
- Web of Science (2012): Indexed yes
- BFI (2011): BFI-level 1
- Scopus rating (2011): SJR 2.433 SNIP 1.663 CiteScore 4.47
- ISI indexed (2011): ISI indexed yes
- Web of Science (2011): Indexed yes
- BFI (2010): BFI-level 1
- Scopus rating (2010): SJR 2.207 SNIP 1.566
- Web of Science (2010): Indexed yes
- BFI (2009): BFI-level 1
- Scopus rating (2009): SJR 2.136 SNIP 1.571
- Web of Science (2009): Indexed yes
- BFI (2008): BFI-level 1
- Scopus rating (2008): SJR 1.914 SNIP 1.455
- Web of Science (2008): Indexed yes
- Scopus rating (2007): SJR 1.839 SNIP 1.566
- Web of Science (2007): Indexed yes
- Scopus rating (2006): SJR 1.98 SNIP 1.654
- Web of Science (2006): Indexed yes
- Scopus rating (2005): SJR 1.718 SNIP 1.56
- Web of Science (2005): Indexed yes
- Scopus rating (2004): SJR 1.833 SNIP 1.691
- Scopus rating (2003): SJR 1.668 SNIP 1.54
- Web of Science (2003): Indexed yes
- Scopus rating (2002): SJR 1.701 SNIP 1.466
- Web of Science (2002): Indexed yes
- Scopus rating (2001): SJR 1.55 SNIP 1.305
- Web of Science (2001): Indexed yes
- Scopus rating (2000): SJR 1.632 SNIP 1.284
The thermodynamic principles of ligand binding in chromatography and biology

In chromatography, macromolecules do not adsorb in the traditional sense of the word but bind to ligands that are covalently bonded to the surface of the porous bead. Therefore, the adsorption must be modelled as a process where protein molecules bind to the immobilised ligands. The paper discusses the general thermodynamic principles of ligand binding. Models of the multi-component adsorption in ion-exchange and hydrophobic chromatography, HIC and RPLC, are developed. The parameters in the models have a well-defined physical significance. The models are compared to the Langmuir model. In the traditional adsorption models, the standard state Gibbs energy change of adsorption does not depend level of occupancy, but when it depends on the level of occupancy it gives rise to an adsorptive behaviour known as cooperativity. The binding of oxygen to haemoglobin is a well-known example from biology but it is also observed in chromatography due to protein-protein interactions. Retention measurements on P-lactoglobulin A demonstrate this. A discussion of salt effects on hydrophobic interactions in precipitation and chromatography of proteins concludes the paper.

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Application of the cubic-plus-association (CPA) equation of state to complex mixtures with aromatic hydrocarbons

The cubic-plus-association (CPA) equation of state is applied to phase equilibria of mixtures containing alcohols, glycols, water, and aromatic or olefinic hydrocarbons. Previously, CPA has been successfully used for mixtures containing various associating compounds (alcohols, glycols, amines, organic acids, and water) and aliphatic hydrocarbons. We show in this work that the model can be satisfactorily extended to complex vapor-liquid-liquid equilibria with aromatic or olefinic hydrocarbons. The solvation between aromatics/olefinics and polar compounds is accounted for. This is particularly important for mixtures containing water and glycols, but less so for mixtures with alcohols. For water/hydrocarbons, a single binary interaction parameter which accounts for the solvation is fitted to the experimental liquid-liquid equilibria (LLE) data. The interaction parameter of the physical term of the model (the Soave-Redlich-Kwong (SRK) equation of state) can be obtained from mixtures with aliphatic hydrocarbons. For mixtures of glycols with aromatic hydrocarbons, two parameters have been fitted to experimental data, one in the physical (SRK) part and one in the association part of the model. Satisfactory liquid-liquid equilibrium predictions are obtained for multicomponent water-alcohol/glycol-aromatic hydrocarbons using solely parameters obtained from binary data.

General information

State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Phase Equilibria and Separation Processes, Center for Energy Resources Engineering
Authors: Folas, G. (Intern), Kontogeorgis, G. (Intern), Michelsen, M. L. (Intern), Stenby, E. H. (Intern)
Pages: 1527-1538
Publication date: 2006
Main Research Area: Technical/natural sciences
Application of the cubic-plus-association equation of state to mixtures with polar chemicals and high pressures

The cubic-plus-association (CPA) equation of state has been previously applied to vapor-liquid, liquid-liquid, and solid-liquid equilibria of mixtures containing associating compounds (water, alcohols, glycols, acids, amines). Although some high-pressure applications have been presented, emphasis was given to low pressures and liquid-liquid equilibria. In this work, CPA is applied to two classes of mixtures containing polar chemicals for which high-pressure data are available: acetone-containing systems and dimethyl ether mixtures. They are of both scientific and industrial importance. Moreover, CPA is applied to high-pressure solid-liquid equilibria (SLE) for alcohol-alkane mixtures. In the case of acetone-hydrocarbon mixtures, satisfactory results are achieved if acetone is allowed to self-associate. Satisfactory high-pressure acetone-water vapor-liquid equilibrium (VLE) is obtained, comparable to conventional models such as MHV2. Very good results are also obtained for multicomponent vapor-liquid-liquid equilibria for mixtures containing gases, water, and dimethyl ether. Finally, it is shown that high-pressure SLE can be predicted based on interaction parameters obtained from low-pressure SLE data.

General information

State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Folas, G. (Intern), Kontogeorgis, G. (Intern), Michelsen, M. L. (Intern), Stenby, E. H. (Intern)
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Publication information

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Scopus rating (2016): CiteScore 3.1 SJR 0.945 SNIP 1.139
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.949 SNIP 1.146 CiteScore 2.87
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.012 SNIP 1.292 CiteScore 2.85
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 0.982 SNIP 1.243 CiteScore 2.6
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.066 SNIP 1.338 CiteScore 2.56
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
Applications of the simplified perturbed-chain SAFT equation of state using an extended parameter table

An equation of state based on perturbation theory, the simplified perturbed-chain statistical associating fluid theory (PC-SAFT) is applied to binary systems that include an extensive number of non-associating compounds. Pure-component parameters of different compounds that are not available in the literature are estimated by correlating vapour-pressure and liquid-density data and by using an interpolation method. PC-SAFT parameters for 200 new compounds are estimated for different families of nonassociating compounds (alkanes, alkenes, alkynes, cycloalkenes, nitroalkanes, polynuclear aromatics, ketones, esters, sulphides, siloxanes, plasticizers, cyclo- and fluorinated-hydrocarbons, etc.). For many different families of compounds, the segment diameter and interaction energy are found to be constant with increasing molar mass, while the segment number increases linearly with molar mass. Using these parameters, simplified PC-SAFT is shown to predict vapour-liquid equilibria successfully for many nonassociating systems and also correlates liquid-liquid equilibria for perfluorohexane-n-alkane systems. In a few cases, a small binary interaction parameter k(12) is needed for the satisfactory correlation of the experimental data. (c) 2006 Elsevier B.V. All rights reserved.

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Tihic, A. (Intern), Kontogeorgis, G. (Intern), von Solms, N. (Intern), Michelsen, M. L. (Intern)
Pages: 29-43
Publication date: 2006
Main Research Area: Technical/natural sciences
The scientific career of one of the most outstanding scientists in molecular thermodynamics, Professor John M. Prausnitz at Berkeley, reflects the change in the agenda of molecular thermodynamics, from hydrocarbon chemistry to biotechnology. To make thermodynamics a frontier for biotechnology will require much dedicated research to demonstrate the needs. Emphasis must be directed towards understanding the processes and the important issues in the development of novel biopharmaceutical products. Following an introduction to indicate the influence it made on oneself and the difference it made, attention will be given to some important thermodynamic issues related to the recovery of biopharmaceuticals, including an outline of the progress in the area of applied thermodynamics of chromatography and its applications at the IVC Research Centre at DTU. (c) 2006 Elsevier B.V. All rights reserved.
Approach suitable for screening estimation methods for critical properties of heavy compounds

A simple theoretical-based correlation of the ratio of the critical temperature to the critical pressure (T_c/p_c) as a function of the van der Waals surface area (Q_s) has been previously developed based on an extensive database of critical data published prior to 1996. The final equation was the following: 

\[ T_c/p_c = 9.0673 + 0.43309(Q_s^{1.3}) + Q_s^{1.95} \]

where \( T_c \) is the critical temperature in kelvin and \( p_c \) is the critical pressure in bar. This correlation is further validated here based on recent experimental data for various families of organic compounds, including some heavy ones (mono- and diacids, alkenes, cyclo/phenylalkanes, and squalane). This and previous validations verify that this correlation has a much broader application range, up to \( T_c/p_c \) ratios of 200, than the data used in its development (compounds with ratios up to 100). It seems that most organic compounds, including the very heavy and complex ones, follow the trend suggested by this equation. This equation can be used for testing existing group-contribution estimation methods. It is shown here that direct comparison of the Joback and Constantinou-Gani methods for two families of compounds (alkenes and carboxylic acids) is in agreement with their validation via the proposed equation. Similar results have been obtained for other compounds. Both group-contribution methods are of equal accuracy for heavy alkenes and acids, provided that experimental boiling point temperatures are available for the Joback method. If such data are not available, e.g., for heavy compounds, the Constantinou-Gani method should be preferred. The proposed correlation does not offer an alternative to group-contribution methods as it only provides a single relationship of the two critical properties. Its universal character, though, and validation for many heavy compounds offer a way to test and compare existing group-contribution methods and, finally, to select the one that best conforms with the proposed correlation. It is recommended that the proposed correlation is indeed used for high molecular weight compounds for which experimental critical properties are typically not available.
A splitting technique for analytical modelling of two-phase multicomponent flow in porous media

In this paper we discuss one-dimensional models for two-phase Enhanced Oil Recovery (EOR) floods (oil displacement by gases, polymers, carbonized water, hot water, etc.). The main result presented here is the splitting of the EOR mathematical model into thermodynamical and hydrodynamical parts. The introduction of a potential associated with one of the conservation laws and its use as a new independent coordinate reduces the number of equations by one. The (n)x(n) conservation law model for two-phase n-component EOR flows in new coordinates is transformed into a reduced (n-1)x(n-1) auxiliary system containing just thermodynamical variables (equilibrium fractions of components, sorption isotherms) and one lifting equation containing just hydrodynamical parameters (phase relative permeabilities and viscosities). The algorithm to solve analytically the problem includes solution of the reduced auxiliary problem, solution of one lifting hyperbolic equation and inversion of the coordinate transformation. The splitting allows proving the independence of phase transitions occurring during displacement of phase relative permeabilities and viscosities. For example, the minimum miscibility pressure (MMP) and transitional tie lines are independent of relative permeabilities and phases viscosities. Relative motion of polymer, surfactant and fresh water slugs depends on sorption isotherms only. Therefore, MMP for gasflood or minimum fresh water slug size providing isolation of polymer/surfactant from incompatible formation water for chemical flooding can be calculated from the reduced auxiliary system. Reduction of the number of equations allows the generation of new analytical models for EOR. The analytical model for displacement of oil by a polymer slug with water drive is presented.

General information
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Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Pires, A. (Ekstern), Bedrikovetsky, P. (Ekstern), Shapiro, A. (Intern)
Pages: 54-67
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BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.56 SJR 0.764 SNIP 1.631
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.801 SNIP 1.652 CiteScore 2.38
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.692 SNIP 1.751 CiteScore 1.95
PC-SAFT (perturbed-chain statistical associating fluid theory) is a novel equation of state, proposed by Gross and Sadowski in 2001 [J. Gross, G. Sadowski, Perturbed-chain SAFT: an equation of state based on a perturbation theory for chain molecules, Ind. Eng. Chem. Res. 40 (2001) 1244]. It is a variant of the SAFT family and has already found several successful applications, especially for polymer and co-polymer solutions at both low and high pressures. Recently, a simplified version of PC-SAFT proposed by von Solms et al. [N. von Solms, M.L. Michelsen, G.M. Kontogeorgis, Computational and physical performance of a modified PC-SAFT equation of state for highly asymmetric and associating mixtures, Ind. Eng. Chem. Res. 42 (2003) 1098.] has been applied to several complex polymer-solvent systems, including vapor-liquid equilibria, liquid-liquid equilibria and gas solubilities for both single-solvent and mixed-solvents (ternary) systems. This manuscript briefly reviews previous successful applications of PC-SAFT, illustrates the capabilities of the model and indicates some problems and limitations in specific areas, especially aqueous systems and blends, as well as challenges that need to be addressed in the future for describing various systems of practical significance. (c) 2006 Elsevier B.V. All rights reserved.
Comparison of the SRK and CPA equations of state for physical properties of water and methanol

Accurate modelling of reservoir fluids containing hydrocarbons, water, and a hydrate inhibitor is an important area for the petroleum industry. Often cubic Equations of State as for example the SRK equation are used. It is desirable that the applied thermodynamic model is applicable not only to calculate phase compositions and saturation conditions but also phase properties like density and heat capacity. Hydrocarbon phase properties can generally be simulated quite accurately using a conventional cubic equation of state with a volume shift parameter. As petroleum reservoir fluids are often produced together with water, properties of water and additives like methanol and glycol is another target area. Being more polar than hydrocarbons, water, alcohols and glycols may require more advanced models for example an association model like CPA (CubicPlus-Association). This type of model has previously been found to be well suited for phase equilibrium calculations on mixtures of hydrocarbons and polar compounds. In this work, SRK (with and without Peneloux volume correction) and CPA are compared for pure water, pure methanol and water-methanol binary mixtures with the purpose of evaluating the performance of the models for associating compounds found in produced reservoir fluids. The properties considered are density, constant pressure heat capacity, velocity of sound, the derivative (partial derivative V/partial derivative P)(T), enthalpy and Joule-Thomson coefficient. It is shown that the CPA model performed better than SRK-Peneloux in most cases and better than SRK without Peneloux correction for all properties considered.

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General information
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Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Lundstrøm, C. (Ekstern), Michelsen, M. L. (Intern), Kontogeorgis, G. (Intern), Pedersen, K. S. (Ekstern), Sørensen, H. (Ekstern)
Pages: 149-157
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Main Research Area: Technical/natural sciences

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Scopus rating (2016): CiteScore 2.33 SJR 0.869 SNIP 1.155
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.874 SNIP 0.998 CiteScore 1.99
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 0.982 SNIP 1.248 CiteScore 2.28
Web of Science (2014): Indexed yes
Comparison of two association models (Elliott-Suresh-Donohue and simplified PC-SAFT) for complex phase equilibria of hydrocarbon-water and amine-containing mixtures

Two Wertheim-based association models, the simplified PC-SAFT and the Elliott-Suresh-Donohue (ESD) equation of state, are compared in this work for the description of vapor-liquid equilibria (VLE) and liquid-liquid equilibria (LLE) in binary systems of aniline, cyclohexylamine (CHA), hydrocarbons, and water. Furthermore, the predictive capabilities of the models are investigated for four ternary systems composed of these components, which exhibit complex liquid-liquid(-liquid) equilibria (LLLE). Various aspects of association models which have an influence in the results are studied for the PC-SAFT equation of state, e.g., the choice of various association schemes for the amines and parametrization of water as well as different approaches for describing solvation. It is shown that simplified PC-SAFT using water parameters estimated in this work can describe successfully water-alkane LLE. In general, both models perform overall similarly for the binary systems, although ESD shows a remarkably good behavior despite its simplicity and the use of only the two-site scheme for all associating compounds. The prediction of the LLE in the ternary systems water + octane + aniline and
water + CHA + aniline is satisfactory whereas larger deviations were obtained for the systems water + octane + CHA and octane + CHA + aniline.
Efficient Reaction Integration for In-Situ Combustion Simulation

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Kristensen, M. R. (Intern), Gerritsen, M. (Ekstern), Thomsen, P. G. (Intern), Michelsen, M. L. (Intern), Stenby, E. H. (Intern)
Publication date: 2006

Host publication information
Title of host publication: 27th International Energy Agency Symposium on Enhanced Oil Recovery
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 192786
Publication: Research - peer-review › Article in proceedings – Annual report year: 2006

Evaluation of the truncated perturbed chain-polar statistical associating fluid theory for complex mixture fluid phase equilibria

Perturbed chain-statistical associating fluid theory (PC-SAFT) was extended rigorously to polar fluids based on the theory of Stell and co-workers [Mol. Phys. 1977, 33, 987]. The new PC-SAFT was simplified to truncated PC-SAFT (tPC-SAFT) so that it can be practical for real polar fluid thermodynamic calculations. In this work, tPC-SAFT is generalized to multicomponent mixtures and evaluated for a wide range of highly nonideal polar mixtures. Binary and ternary mixtures of dipolar, quadrupolar, and/or associating fluids are examined. Vapor-liquid and liquid-liquid equilibria at low and high pressures are calculated. Comparisons against PC-SAFT calculations are made. It is shown that tPC-SAFT is an accurate model for polar fluid mixture phase equilibria.

General information
State: Published
Organisations: Center for Energy Resources Engineering, Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering
Authors: Karakatsani, E. (Intern), Kontogeorgis, G. (Intern), Economou, I. (Intern)
Pages: 6063-6074
Publication date: 2006
Main Research Area: Technical/natural sciences

Publication information
Journal: Industrial & Engineering Chemistry Research
Volume: 45
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ISSN (Print): 0888-5885
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<td>2.04 CiteScore 2.04</td>
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<td>2003</td>
<td>BFI-level 2</td>
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<td>BFI-level 2</td>
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<td>2002</td>
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<td>SJR 1.146 SNIP 1.165</td>
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<td>BFI-level 2</td>
<td>2.04 CiteScore 2.04</td>
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<td>2001</td>
<td>BFI-level 2</td>
<td>Indexed yes</td>
<td>SJR 1.047 SNIP 1.165</td>
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<td>BFI-level 2</td>
<td>2.04 CiteScore 2.04</td>
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<td>2000</td>
<td>BFI-level 2</td>
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<td>BFI-level 2</td>
<td>2.04 CiteScore 2.04</td>
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<td>1999</td>
<td>BFI-level 2</td>
<td>Indexed yes</td>
<td>SJR 1.146 SNIP 1.165</td>
<td>Indexed yes</td>
<td>BFI-level 2</td>
<td>2.04 CiteScore 2.04</td>
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Original language: English
DOIs:
Experimental investigation of the diffusion coefficients in porous media by application of X-ray computer tomography

The present work describes a new experimental method that makes it possible to investigate diffusion coefficients in a porous medium. The method is based on application of X-ray computed tomography (CT). The general applicability of this method for the determination of diffusion coefficients is demonstrated. A series of such experiments was carried out. Several samples of carbonaceous and sandstone rock were investigated. The diffusion coefficients in porous media were determined by measuring the concentration of salt in different slices of a sample as a function of time. In cases where stable values of diffusion coefficients were obtained (all samples except for one highly heterogeneous sample), these values served for the determination of the tortuosity-porosity factors for a given type of porous medium.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Phase Equilibria and Separation Processes, Center for Energy Resources Engineering
Authors: Zhelezny, P. (Intern), Shapiro, A. (Intern)
Pages: 275-288
Publication date: 2006
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Porous Media
Volume: 9
Issue number: 4
ISSN (Print): 1091-028X
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 0.492 SNIP 0.744 CiteScore 1.22
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.456 SNIP 0.789 CiteScore 1.05
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.365 SNIP 0.654 CiteScore 0.81
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.295 SNIP 0.488 CiteScore 0.6
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.385 SNIP 0.617 CiteScore 0.65
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.388 SNIP 0.943 CiteScore 0.81
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.411 SNIP 0.689
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.323 SNIP 0.621
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.472 SNIP 0.509
Scopus rating (2007): SJR 0.322 SNIP 0.623
Scopus rating (2006): SJR 0.671 SNIP 0.653
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.07 SNIP 1.4
High-pressure viscosity behavior of x \text{1,1,1,2-tetrafluoroethane (HFC-134a)+(1-x) triethylene glycol dimethylether (TriEGDME) mixtures: Measurements and modeling}

In this work new dynamic viscosity measurements for binary mixtures containing a refrigerant (HFC-134a, CF3CH2F) and a lubricant (TriEGDME, CH3O(CH2OCH2)(3)CH3) are reported. The measurements were carried out at temperatures between 293.15 and 373.15 K and pressures from 10 to 100 MPa, for two mole fractions x(HFC) = 0.3427 and 0.5940 (a total of 100 experimental values). Since lubricants and refrigerants are in two different thermodynamic states at atmospheric pressure and ambient temperature, an especially designed falling-body viscometer has been used to perform the measurements. The data obtained for this binary system have been used to test the ability of several viscosity models having different origins and theoretical backgrounds. The considered models range from simple mixing rules, through empirical correlations, such as the self-referencing model and the LBC model, to recent approaches with a physical and theoretical background, such as the hard-sphere scheme, the free-volume model, and the friction theory.

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Monsalvo, M. A. (Intern), Baylaucq, A. (Ekstern), Cisneros, S. (Intern), Boned, C. (Ekstern)
Pages: 70-79
Publication date: 2006
Main Research Area: Technical/natural sciences

Publication information
Journal: Fluid Phase Equilibria
Volume: 247
Issue number: 1-2
ISSN (Print): 0378-3812
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 2.33 SJR 0.869 SNIP 1.155
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.874 SNIP 0.998 CiteScore 1.99
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 0.982 SNIP 1.248 CiteScore 2.28
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.007 SNIP 1.274 CiteScore 2.31
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.152 SNIP 1.286 CiteScore 2.31
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
Increasing the computational speed of flash calculations with applications for compositional, transient simulations

Approaches are presented for reducing the computation time spent on flash calculations in compositional, transient simulations. In a conventional flash calculation, the majority of the simulation time is spent on stability analysis, even for systems far into the single-phase region. A criterion has been implemented for deciding when it is justified to bypass the stability analysis. With the implementation of the developed time-saving initiatives, it has been shown for a number of compositional, transient pipeline simulations that a reduction of the computation time spent on flash calculations by approximately 85 to 90% can be achieved.
Liquid-liquid equilibria for binary and ternary systems containing glycols, aromatic hydrocarbons, and water: Experimental measurements and modeling with the CPA EoS

Liquid-liquid equilibrium data of four binary glycol + aromatic hydrocarbon systems and three ternary systems containing water have been measured at atmospheric pressure. The measured systems are monoethylene glycol (MEG) + benzene or toluene, triethylene glycol (TEG) + benzene or toluene, MEG + water + benzene, MEG + water + toluene, and TEG + water + toluene. The binary systems are correlated with the Cubic-Plus-Association (CPA) equation of state while the ternary systems are predicted from interaction parameters obtained from the binary systems. Very satisfactory liquid-liquid equilibrium correlations are obtained for the binary systems using temperature-independent interaction parameters, while adequate predictions are achieved for multicomponent water + glycol + aromatic hydrocarbons systems when accounting for the solvation between the aromatic hydrocarbons and glycols or water.
(Liquid plus liquid) equilibria of binary polymer solutions using a free-volume UNIQUAC-NRF model

In this work, a modified free-volume (FV) model based on the UNIQUAC-Nonrandom factor (UNIQUAC-NRF) model developed by Haghtalab and Asadollahi was proposed. While the combinatorial part of the proposed model for activity coefficient takes the same form as that of the entropic free-volume (entropic-FV) model, the residual part is similar to that of the UNIQUAC-NRF model. The proposed model, i.e., the FV-UNIQUAC-NRF model overcomes the main shortcoming of the original UNIQUAC-NRF model in predicting the lower critical solution temperature (LCST) for polymer solutions. The appearance of the LCST is believed to be attributed to the existence of the free volume differences between polymer and solvent molecules. Thus, the models without considering such differences fail to predict the LCST behavior of polymer solutions. The proposed model was applied to correlate the experimental data of (liquid + liquid) equilibria (LLE) for a number of binary polymer solutions at various temperatures. The values for the binary characteristic energy parameters for the proposed model and the FV-UNIQUAC model along with their average relative deviations from the experimental data were reported. It should be stated that the binary polymer solutions studied in this work were considered as monodisperse. The results obtained from the FV-UNIQUAC-NRF model were compared with those obtained from the FV-UNIQUAC model. The results of the proposed model show that the FV-UNIQUAC-NRF model can accurately correlate the experimental data for LLE of polymer solutions studied in this work. Also the error produced from the FV-UNIQUAC-NRF model show the slightly better accuracy in comparison with that from the FV-UNIQUAC model. The clear advantage of the proposed model, contrary to the original UNIQUAC-NRF model, is its capability in predicting the LCST for binary polymer solutions.

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Radfarnia, H. (Ekstern), Ghotbi, C. (Ekstern), Taghikhani, V. (Ekstern), Kontogeorgis, G. (Intern)
Pages: 923-928
Publication date: 2006
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Chemical Thermodynamics
Volume: 38
Issue number: 7
ISSN (Print): 0021-9614
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.64 SJR 1 SNIP 1.163
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.075 SNIP 1.091 CiteScore 2.29
Web of Science (2015): Indexed yes
Modeling of CO2 absorber using an AMP solution

Abstract: An explicit model for carbon dioxide (CO2) solubility in an aqueous solution of 2-amino-2-methyl-1-propanol (AMP) has been proposed and an expression for the heat of absorption of CO2 has been developed as a function of loading and temperature. A rate-based steady-state model for CO2 absorption into an AMP solution has been proposed, using both the proposed expression for the CO2 solubility and the expression for the heat of absorption along with an expression for the enhancement factor and physicochemical data from the literature. The proposed model has successfully been applied to absorption of CO2 into an AMP solution in a packed tower and validated against pilot-plant data from the literature. (c) 2006 American Institute of Chemical Engineers.

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Gabrielsen, J. (Intern), Michelsen, M. L. (Intern), Stenby, E. H. (Intern), Kontogeorgis, G. (Intern)
Pages: 3443-3451
Scopus rating (2001): SJR 2.16 SNIP 2.077
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 1.953 SNIP 1.76
Scopus rating (1999): SJR 1.55 SNIP 1.74
Original language: English
DOI:
10.1002/aic.10963
Source: orbit
Source-ID: 191131
Publication: Research - peer-review › Journal article – Annual report year: 2006

Multicomponent Adsorption Approaches to Modeling Adsorption Equilibria

General information
State: Published
Organisations: CERE – Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Shapiro, A. (Intern), Stenby, E. H. (Intern)
Number of pages: 8,032
Pages: 4180-4189
Publication date: 2006

On the Process of Gas Liberation in Porous Media
The aim of the present work is an experimental and computational analysis of the effect of gas liberation in a porous medium. The experiments are based on application of X-ray computed tomography (CT). A series of experiments on slow gas liberation was carried out. A mathematical model of the liberation process was developed based on the theory of differential depletion in the presence of a porous medium. The porous samples involved were low-permeable North Sea core plugs and artificial glass core. The results of the experiments indicate rather uniform gas production in different parts of the samples. The results of the calculations indicate noticeable, although not extreme, lowering of the bubble point pressure (0.12-0.18 MPa) and decreased production of gas, compared to the depletion carried out in a PVT cell.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Phase Equilibria and Separation Processes, Center for Energy Resources Engineering
Authors: Zhelezny, P. (Intern), Shapiro, A. (Intern), Vu, D. T. (Intern), Stenby, E. H. (Intern)
Pages: 503-521
Publication date: 2006
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Porous Media
Volume: 9
Issue number: 6
ISSN (Print): 1091-028X
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Predicting enhanced absorption of light gases in polyethylene using simplified PC-SAFT and SAFT-VR

Absorption of light gases in polyethylene (PE) is studied using two versions of the Statistical Associating Fluid Theory (SAFT): SAFT for chain molecules with attractive potentials of variable range (VR) and simplified perturbed-chain (PC) SAFT. Emphasis is placed on the light gases typically present during ethylene polymerisation in the gas-phase reactor (GPR) process. The two approaches are validated using experimental binary-mixture data for gas absorbed in PE, and predictions are made for mixtures of more components. For most cases studied both SAFT versions perform equally well. For the case of ternary mixtures of two gases with PE, it is predicted that the less-volatile of the two gases acts to enhance the absorption of the more-volatile gas, while the more-volatile gas inhibits the absorption of the less-volatile gas. This general behaviour is also predicted in mixtures containing more gases, such as typical reactor mixtures. The magnitude of the effect may vary considerably, depending on the relative proximity of the gas-mixture saturation pressure to the reactor pressure; for example it is predicted that the absorption of ethylene may be approximately doubled if diluent gases, propane or nitrogen, are partially or completely replaced by less-volatile butane or pentane for a reactor pressure similar to 2 MPa. In the case of a co-polymerisation reaction, it is predicted that increases in absorption of both co-monomers may be obtained in roughly equal proportion. Our findings cast light on the so-called co-monomer effect, in which substantial increases in the rate of ethylene polymerisation are observed in the presence of hexene co-monomer, while suggesting that the effect is more general and not restricted to co-monomer. For example, similar rate increases may be expected in the presence of, e.g., pentane instead of hexene, but without the change in the branch structure of the produced polymer that is inevitable when the amount of co-monomer is increased. (c) 2006 Elsevier B.V. All rights reserved.

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Prediction of mineral scale formation in geothermal and oilfield operations using the Extended UNIQUAC model - Part II. Carbonate-scaling minerals

Two additional parameters to account for the pressure dependency of solubility are added to the Extended UNIQUAC model presented by Thomsen and Rasmussen (1999). The improved model has been used for correlation and prediction of vapor-liquid-solid equilibrium for different carbonate systems (CaCO₃, MgCO₃, BaCO₃ and SrCO₃) causing scale problems. The solubility of NaCl and CO₂ in pure water, and the solubility of CO₂ in solutions of different salts (NaCl and Na₂SO₄) have also been correlated. The temperature and pressure range covered is from 0 to 250°C and from 1 to 1000 bar, respectively. The results show that the Extended UNIQUAC model, with the proposed pressure parameters, is able to represent binary (NaCl-H₂O, MCO₃-H₂O and CO₂-H₂O), ternary (MCO₃-CO₂-H₂O, CO₂-NaCl-H₂O and CO₂-Na₂SO₄-H₂O) and quaternary (CO₂-NaCl-Na₂SO₄-H₂O) solubility data within the experimental accuracy in the temperature range from 0 to 250°C, and the pressure range from 1 to 1000 bar. M stands for Ca²⁺, Mg²⁺, Ba²⁺ and Sr²⁺.

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Villafafila, A. (Intern), Thomsen, K. (Intern), Stenby, E. H. (Intern)
Pages: 239-284
Publication date: 2006
Main Research Area: Technical/natural sciences

Publication information
Journal: Geothermics
Volume: 35
Issue number: 3
ISSN (Print): 0375-6505
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.67 SJR 0.943 SNIP 1.417
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.344 SNIP 1.987 CiteScore 2.99
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.924 SNIP 3.002 CiteScore 3.61
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.851 SNIP 2.423 CiteScore 3.08
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Prediction of viscosities and surface tensions of fuels using a new corresponding states model

While some properties of diesels are cheap, easy and fast to measure, such as densities, others such as surface tensions and viscosities are expensive and time consuming. A new approach that uses some basic information such as densities to predict viscosities and surface tensions is here proposed using a Corresponding states model previously developed for the accurate estimation of several thermophysical properties of pure and mixed n-alkanes. This approach is tested with good results in five petroleum distillation cuts from crudes of different sources (North Sea, Africa and Middle East). (C) 2005 Elsevier Ltd. All rights reserved.
Equations of state that incorporate the Wertheim association expression are more difficult to apply than conventional pressure explicit equations, because the association term is implicit and requires solution for an internal set of composition variables. In this work, we analyze the convergence behavior of different solution methods and demonstrate how a simple and efficient, yet globally convergent, procedure for the solution of the equation of state can be formulated.
Scale-up of chromatographic ion-exchange processes in biotechnology

The van Deemter equation has been used to derive a rule of thumb guideline for scaling. The scaling is done by the concept of time scales. The time scales are kept identical for all the columns by scaling the flow rate to the total void volume and the load to the amount of the media. The verification of theoretical background for the linear gradient elution is reported. The results demonstrate that the gradient retention behaviour of protein is independent of the column aspect ratio, but it's a function of the initial salt concentration and the gradient slope. (c) 2006 Elsevier B.V. All rights reserved.

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Al-Jibbouri, S. (Intern)
Pages: 135-142
Publication date: 2006
Main Research Area: Technical/natural sciences

Publication Information
Journal: Journal of Chromatography A
Volume: 1116
Issue number: 1-2
ISSN (Print): 0021-9673
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.97 SJR 1.462 SNIP 1.295
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.713 SNIP 1.395 CiteScore 4.03
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.825 SNIP 1.509 CiteScore 4.28
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 2.017 SNIP 1.616 CiteScore 4.6
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 2.31 SNIP 1.703 CiteScore 4.6
ISI indexed (2012): ISI indexed yes
Solid-liquid equilibria for the binary mixtures 1,4-xylene plus ethylbenzene and 1,4-xylene plus toluene (vol 191, pg 1017, 2004)

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Phase Equilibria and Separation Processes, Center for Energy Resources Engineering
Authors: Huyghe, R. (Intern), Rasmussen, P. (Intern), Thomsen, K. (Intern)
Pages: 272-272
Publication date: 2006
Main Research Area: Technical/natural sciences

Publication information
Journal: Chemical Engineering Communications
Volume: 193
Issue number: 2
ISSN (Print): 0098-6445
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
Study of Pressure and Temperature Effects on Asphaltene Stability in Presence of CO2

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Verdier, S. C. R. (Intern), Carrier, H. (Ekstern), Andersen, S. I. (Intern), Daridon, J. (Ekstern)
Pages: 1584-1590
Publication date: 2006
Main Research Area: Technical/natural sciences

Publication information
Journal: Energy & Fuels
Volume: 20
ISSN (Print): 0887-0624
Ten years with the CPA (Cubic-Plus-Association) equation of state. Part 1. Pure compounds and self-associating systems

CPA (Cubic-Plus-Association) is an equation of state that is based on a combination of the Soave-Redlich-Kwong (SRK) equation with the association term of the Wertheim theory. The development of CPA started in 1995 as a research project funded by Shell (Amsterdam), and the model was first published in 1996. Since then, it has been successfully applied to a variety of complex phase equilibria, including mixtures containing alcohols, glycols, organic acids, water, and hydrocarbons. Focus has been placed on cases of industrial importance, e.g., systems with gas-hydrate inhibitors (methanol, glycols), glycol regeneration and gas dehydration units, oxygenate additives in gasoline, alcohol separation, etc. This manuscript, which is the first of a series of two papers, offers a review of previous applications and illustrates current focus areas related to the estimation of pure compound parameters, alcohol-hydrocarbon vapor-liquid equilibria (VLE) and solid-liquid equilibria (SLE), as well as aqueous systems. The capabilities and limitations of CPA are discussed and suggestions for extension of the model to systems not covered in this work are provided.
General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Kontogeorgis, G. (Intern), Michelsen, M. L. (Intern), Folas, G. (Intern), Derawi, S. (Intern), von Solms, N. (Intern), Stenby, E. H. (Intern)
Pages: 4855-4868
Publication date: 2006
Main Research Area: Technical/natural sciences
Publication information
Journal: Industrial & Engineering Chemistry Research
Volume: 45
Issue number: 14
ISSN (Print): 0888-5885
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.1 SJR 0.945 SNIP 1.139
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Web of Science (2015): Indexed yes
Scopus rating (2015): SJR 0.949 SNIP 1.146 CiteScore 2.87
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.012 SNIP 1.292 CiteScore 2.85
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 0.982 SNIP 1.243 CiteScore 2.6
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
ISI indexed (2012): ISI indexed yes
Scopus rating (2012): SJR 1.066 SNIP 1.338 CiteScore 2.56
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
ISI indexed (2011): ISI indexed yes
Scopus rating (2011): SJR 1.086 SNIP 1.24 CiteScore 2.58
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.047 SNIP 1.165
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.002 SNIP 1.164
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 1.142 SNIP 1.267
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.105 SNIP 1.239
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.035 SNIP 1.204
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 0.993 SNIP 1.241
Web of Science (2005): Indexed yes
Ten years with the CPA (Cubic-Plus-Association) equation of state. Part 2. Cross-associating and multicomponent systems

In this second article of the review on the applications of the CPA (Cubic-Plus-Association) equation of state, the focus is placed on cross-associating systems. Various such mixtures are investigated, including (i) systems with two self-associating compounds (e.g., water-alcohol systems or glycols, mixtures with organic acids, or two alcohols) but also binaries with only one self-associating substance, where solvation is expected (e.g., CO2 or styrene with water). The method of accounting for cross-association (combining rules) and the association scheme of alcohols are investigated. Finally, the manuscript concludes with a summary of current capabilities and limitations of CPA and a list of future challenges.

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Kontogeorgis, G. (Intern), Michelsen, M. L. (Intern), Folas, G. (Intern), Derawi, S. (Intern), von Solms, N. (Intern), Stenby, E. H. (Intern)
Pages: 4869-4878
Publication date: 2006
Main Research Area: Technical/natural sciences

Publication information
Journal: Industrial & Engineering Chemistry Research
Volume: 45
Issue number: 14
ISSN (Print): 0888-5885
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.1 SJR 0.945 SNIP 1.139
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.949 SNIP 1.146 CiteScore 2.87
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.012 SNIP 1.292 CiteScore 2.85
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 0.982 SNIP 1.243 CiteScore 2.6
The McMillan-Mayer framework and the theory of electrolyte solutions

In electrolyte thermodynamics one often speaks of two thermodynamic frameworks; the Lewis-Randall framework (characterised by temperature, pressure, and mole numbers) and the McMillan-Mayer framework (characterised by temperature, total volume, solute mole numbers, and solvent chemical potential). However, there is only one framework in thermodynamics; the apparent difference between the two ‘frameworks’ is, in electrolyte thermodynamics, due to the change in the pressure caused by the charging process at constant volume and solvent chemical potential. The so-called McMillan-Mayer framework is set in the context of the classical thermodynamics and the use of it is exemplified by the Debye-Huckel theory. The so-called McMillan-Mayer framework is superfluous when the thermodynamics of the electrolyte solutions is described by the Helmholtz energy functions. (c) 2006 Elsevier B.V. All rights reserved.

General information

State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Thermodynamic modeling of acidic gas solubility in aqueous solutions of MEA, MDEA and MEA-MDEA blends

The thermodynamic framework that was developed in a previous work [Vrachnos et al. Ind. Eng. Chem. Res. 2004, 43, 2798] for the description of chemical and vapor-liquid equilibria of carbon dioxide, hydrogen sulfide, and their mixtures in aqueous methyl diethanolamine (MDEA) solutions is revised and extended in this study to the absorption of carbon dioxide into aqueous monoethanolamine (MEA) solutions and aqueous MDEA-MEA blends. The results of the model are compared with experimental data taken from the literature. Very satisfactory predictions of acidic gas vapor-liquid equilibrium over MDEA, MEA, and their blends at various concentrations, acidic gas loadings, and temperatures are obtained.

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Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Vrachnos, A. (Ekstern), Kontogeorgis, G. (Intern), Voutsas, E. (Ekstern)
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Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.012 SNIP 1.292 CiteScore 2.85
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 0.982 SNIP 1.243 CiteScore 2.6
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Scopus rating (2012): SJR 1.066 SNIP 1.338 CiteScore 2.56
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Vapor-liquid, liquid-liquid and vapor-liquid-liquid equilibrium of binary and multicomponent systems with MEG modeling with the CPA EoS and an EoS/G(E) model

The cubic-plus-association (CPA) EoS is applied to multicomponent multiphase equilibria of systems containing MEG as a hydrate inhibitor. It is shown that the model provides very satisfactory prediction of the phase behavior for the systems tested. A more conventional engineering model for handling associating and polar molecules, an EoS/G(E) model is also tested, both for binary and multicomponent systems, and compared to the performance of the CPA EoS. It is found that the performance of CPA is overall superior while using fewer interaction parameters than the EoS/G(E) approach. (c) 2006 Elsevier B.V. All rights reserved.
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Web of Science (2015): Indexed yes
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Scopus rating (2011): SJR 1.034 SNIP 1.234 CiteScore 2.26
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BFI (2010): BFI-level 2
Scopus rating (2010): SJR 0.986 SNIP 1.317
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Scopus rating (2009): SJR 1.133 SNIP 1.164
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.227 SNIP 1.09
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.031 SNIP 1.151
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.034 SNIP 1.245
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Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 0.985 SNIP 1.349
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 1.193 SNIP 1.301
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 0.722 SNIP 1.101
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 0.966 SNIP 1.284
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 0.87 SNIP 0.898
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A model for estimating CO2 solubility in aqueous alkanolamines

Partial pressures of carbon dioxide (CO2) over aqueous solutions of monoethanolamine (MEA), diethanolamine (DEA), and N-methyldiethanolamine (MDEA) have been correlated using a simple approach where only one chemical equilibrium reaction is taken into account and assuming ideal gas and ideal liquid properties. The approach combines the Henry's law constant and the chemical reaction equilibrium constant for the formation of carbamate for primary and secondary alkanolamines (MEA, DEA) or bicarbonate for tertiary alkanolamines (MDEA), resulting in an explicit expression for calculating the partial pressure of CO2 over an aqueous alkanolamine solution. Accurate values for the partial pressure of CO2 are obtained for a limited loading, temperature, and pressure range that is useful in modeling CO2 capture from coal-fired power plants. Heat of absorption values derived from the model agree with experimental data from the literature.
A modified free-volume-based model for predicting vapor-liquid and solid-liquid equilibria for size asymmetric systems

The main purpose of this work is to present a free-volume combinatorial term in predicting vapor-liquid equilibrium (VLE) and solid-liquid equilibrium (SLE) of polymer/solvent and light and heavy hydrocarbon/hydrocarbon mixtures. The proposed term is based on a modification of the original Freed Flory-Huggins model, replacing the molar volume with a free-volume (FV) term. Using an extensive database for athermal polymer solutions at finite dilution, the single parameter of the model has been well adjusted. The results obtained from the model proposed in this work were favorably compared with those obtained from the well-established entropic-FV based models, i.e., the original entropic-FV (EFV) and the modified entropic-FV (MEFV) models. The results were also compared with those of the original UNIFAC-FV model as well as a modified UNIFAC-FV model, Kannan-FV, recently proposed model by Karman et al. The results obtained from the proposed model showed that better improvement can be attained for the polymer systems with energetic interactions as well as for VLE and SLE study of heavy alkane solutes in light alkane solvents. This observation can be further verified by comparison of the results obtained from the proposed model with those of the molecular simulation data. (c) 2005 Elsevier B.V. All rights reserved.

General information
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Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
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Application of Advanced Thermodynamic Models for Complex Fluids and Reservoirs

General information
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Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Yan, W. (Intern), Kontogeorgis, G. (Intern), Stenby, E. H. (Intern)
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Source-ID: 188060
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Application of the cubic-plus-association (CPA) equation of state to cross-associating systems
The cubic-plus-association (CPA) equation of state (EoS) is applied, using different combining rules, to vapor-liquid equilibria (VLE) and liquid-liquid equilibria (LLE) of alcohol-water systems. It is demonstrated that the Elliott combining rule (ECR) with a common temperature-independent interaction parameter provides very adequate VLE correlations over extended temperature and pressure ranges, yielding also a very satisfactory description of the azeotropic behavior. LLE of heavy alcohol-water systems is best described with the CR-1 combining rule and a single interaction parameter. Satisfactory predictions of multicomponent, multiphase equilibria of water-alcohol-alkane systems at various conditions are achieved using solely one interaction parameter per binary. A study of the dominant binary systems for the prediction of the multicomponent systems demonstrates that both the binary alcohol-water and alcohol-hydrocarbon systems are crucial for the prediction of the partition coefficients of alcohols. Finally, the CPA EoS combined with a model for the solid-complex formation can successfully describe solid-liquid equilibria of glycol/methanol-water systems including the description of the solid-complex phase, which is known to exist at intermediate concentrations.

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Organisations: Department of Chemical and Biochemical Engineering, Center for Phase Equilibria and Separation Processes, Center for Energy Resources Engineering
Authors: Folas, G. (Intern), Gabrielsen, J. (Intern), Michelsen, M. L. (Intern), Stenby, E. H. (Intern), Kontogeorgis, G. (Intern)
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Web of Science (2016): Indexed yes
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Biothermodynamics - a Tool for a More Efficient Process Development

General information
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Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Calorimetric Evidence about the Application of the Concept of CMC to Asphaltene Self-Association

For many years, the concept of critical micellar concentration (CMC) has been projected from surfactant science into asphaltene science. There are several similarities between these two species, such as the stabilization of water-in-oil emulsions and surface activity, which suggested that asphaltenes may also have a concentration at which self-association occurs (CMC). This article presents evidence found by calorimetry and spectroscopic techniques, that suggest that this concept may not be adequate for asphaltene self-association in toluene solutions. Isothermal titration calorimetry has been widely used in surfactant science to determine both the CMC and the enthalpy of micellation of many surfactants. The concentration interval could be divided into three regions: monomer region, micellation region, and micelle region. The absence of the first region (monomer) in the concentration range usually found in the literature as the CMC region of asphaltenes indicates that this concept is not appropriate for asphaltene self-association. Tests were performed down to concentrations of 34ppm without any sign of a critical micellization or aggregation concentration. Based on the various techniques applied, which also include IR and fluorescence spectroscopy, it is concluded that asphaltenes do not exhibit CMC behavior. Instead, the association of asphaltenes is believed to occur step wise. This is not in disagreement with the fact that the aggregates may end up having a definite size.
Comments on "Predictions of activity coefficients of nearly athermal binary mixtures using cubic equations of state"

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Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
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BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.1 SJR 0.945 SNIP 1.139
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
A field experiment was performed in a sandy vadose zone, studying the fate of an emplaced fuel-NAPL source, composed of 13 hydrocarbons and a tracer. The UNIFAC model was used to test the nonideal behavior of the source, and the numerical model MIN3P was used for assessing the effect of biodegradation on source evolution. The diffusive loss to the surrounding vadose zone and the atmosphere created temporary gradients in mole fractions of the individual compounds within the source NAPL. The evolution of the source composition corresponded in general with expectations based on
Raoult's Law, with the exception that the mole fractions of aromatic compounds in the source NAPL decreased faster than fractions of aliphatic compounds of similar volatility. Calculation of activity coefficients (gamma) using the UNIFAC model implied nonideal conditions, with composition-dependent gamma's different from 1. Positive deviations were calculated for the aromatic compounds. The effect of biodegradation on source depletion, evaluated by numerical modeling, was greater for the aromatic as compared to the aliphatic compounds. Hence, the faster depletion of the aromatic relative to aliphatic compounds of similar volatility is both a result of the nonideality of the mixture and a result of partitioning and biodegradation in the pore-water. Vapor concentrations of the compounds in the source were in reasonable agreement with predictions based on the modified Raoult's Law with the UNIFAC predicted gamma's and the NAPL composition for the most volatile compounds. For the less volatile compounds, the measured vapor concentrations were lower than predicted with the largest deviations for the least volatile compounds. This field experiment illustrated that nonideal behavior and bioenhanced source depletion need to be considered at multicomponent NAPL spill sites.
Correlation and prediction of environmental properties of alcohol ethoxylate surfactants using the UNIFAC method

Environmental properties of one type of nonionic surfactants, the alcohol ethoxylates (polyoxyethylene alcohols), are predicted using the UNIFAC (universal quasi-chemical functional group activity coefficient) method. Various properties are considered; the octanol-water partition coefficient (Kow), the bioconcentration factor (BCF), and the toxicity. Kow values of alcohol ethoxylates are difficult to measure. Existing methods such as those in commercial software like ACD/ClogP and KowWin have not been applied to surfactants, and they fail for heavy alcohol ethoxylates (alkyl carbon numbers above 12). Thus, the Kow values are predicted here via UNIFAC and compared to the few available experimental data. Based on the predicted Kow values, a correlation between Kow and hydrophilic-lipophilic balance (HLB) is established because HLB is a widely used parameter in surfactant applications. Finally, BCF and toxicity of alcohol ethoxylates are correlated with their Kow. The proposed approach can be extended to other families of nonionic surfactants.

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Organisations: Food Production Engineering, Department of Chemical and Biochemical Engineering, Center for Phase Equilibria and Separation Processes, Center for Energy Resources Engineering
Authors: Cheng, H. (Intern), Kontogeorgis, G. (Intern), Stenby, E. H. (Intern)
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Density and viscosity behavior of a North Sea crude oil, natural gas liquid, and their mixtures

The friction theory (f-theory) for viscosity modeling, combined with a recently developed characterization procedure, which includes an accurate method to describe the fluid mass distribution, commonly used cubic equations of state, and a Peneloux-type volume translation scheme, have been shown to accurately model the saturation pressures, densities, and viscosities of petroleum systems ranging from natural gases to heavy crude oils. The applicability of this overall modeling technique to reproduce measured bubble points, densities, and viscosities of a North Sea crude oil, a natural gas liquid, and their mixtures has been investigated. The approach has been successfully applied to the modeling of the experimental data of these fluid systems to within an acceptable accuracy.
Density and viscosity modeling and characterization of heavy oils

Viscosity and density are key properties for the evaluation, simulation, and development of petroleum reservoirs. Previously, the friction theory (f-theory) was shown to be capable of delivering simple and accurate viscosity models for petroleum reservoir fluids with molecular weights up to similar to 200 g/mol and viscosities up to similar to 10 mPa s, under usual reservoir conditions. As a basis, the f-theory approach requires a compositional characterization procedure that is used in conjunction with a van der Waals type of equation of state (EOS). This is achieved using simple cubic EOSs, which are widely used within the oil industry. Further work also established the basis for extending the approach to heavy oils. Thus, in this work, the extended f-theory approach is further discussed with the study and modeling of a wider set of representative heavy reservoir fluids with viscosities up to thousands of mPa center dot s. Essential to the presented extended approach for heavy oils is, first, achievement of accurate P nu T results for the EOS-characterized fluid. In particular, it has been determined that, for accurate viscosity modeling of heavy oils, a compressibility correction in the way that the EOS is coupled to the viscosity model is required. Thus, in this work, the f-theory potential for the viscosity modeling and prediction of heavy reservoir fluids is further discussed.

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Web of Science (2016): Indexed yes
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Scopus rating (2015): CiteScore 3.34
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 3.3
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 3.52
Density measurements under pressure for the binary system 1-propanol plus toluene

The density of the binary system composed of 1-propanol and toluene has been measured under pressure using a vibrating-tube densimeter. The measurements have been performed for four different compositions as well as the pure compounds at four temperatures in the range of (303.15 to 333.15) K and seven isobars up to 30 MPa. The uncertainty of the reported densities is less than 0.05%. The measured data has been used to study the influence of temperature, pressure, and composition on the isothermal compressibility and the isobaric thermal expansivity as well as the excess molar volume, which shows a complex sigmoid behavior involving both positive and negative values. This complex behavior has been interpreted as the result of changes in the free volume due to volume expansion and compressibility as a result of the breaking of hydrogen bonds of the self-associating alcohol molecules but also due to the electron donor-acceptor-type formation of hydrogen bonding between the hydroxyl group of 1-propanol and the pi electrons of toluene because aromatic hydrocarbons can act as electron donors.

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Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.868 SNIP 0.966 CiteScore 1.96
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BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.021 SNIP 1.208 CiteScore 2.22
Web of Science (2014): Indexed yes
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BFI (2012): BFI-level 1
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ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.862 SNIP 0.988 CiteScore 1.8
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.054 SNIP 1.299
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.313 SNIP 1.037
Web of Science (2009): Indexed yes
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Scopus rating (2008): SJR 1.505 SNIP 1.186
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Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.146 SNIP 1.33
Web of Science (2006): Indexed yes
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Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 0.897 SNIP 1.205
Scopus rating (2003): SJR 1.054 SNIP 1.157
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 0.661 SNIP 1.062
Web of Science (2002): Indexed yes
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Web of Science (2001): Indexed yes
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Density measurements under pressure for the binary system (ethanol plus methylcyclohexane)

The density of the asymmetrical binary system composed of ethanol and methylcyclohexane has been measured under pressure using a vibrating tube densimeter. The measurements have been performed for eight different compositions as well as the pure compounds at eight temperatures in the range 283.15 K to 353.15 K and ten isobars up to 45 MPa. The uncertainty for the reported densities is estimated to be 0.1 kg m\(^{-3}\). A non-monotonal behavior involving a minimum in the density versus composition has been found for this binary system. The measured data have been used to study the behavior and influence of temperature, pressure and composition on the excess molar volume, the isothermal compressibility, and the isobaric thermal expansion, revealing that a volume expansion occurs for this binary system. The results have been interpreted as due to changes in the intermolecular distances or free-volume, disruption of the order molecular structure and the breaking of hydrogen bonds within the self-associating alcohol. (c) 2005 Elsevier Ltd. All rights reserved.
Development and application of a three-parameter RK-PR equation of state

In this work, we confirm the somehow previously expressed but not widespread idea that the limitations of cubic equations of state like Soave-Redlich-Kwong equation (SRK) or Peng-Robinson equation (PR) are a consequence of their two-parameter density dependence rather than of their empiric character. Moreover, it is shown that when combined with a simple generalized van der Waals attraction term, the van der Waals repulsion is more capable than the Carnahan-Starling term to follow the PVT behaviour of real fluids and, in particular, that the generalized Redlich-Kwong-Peng-Robinson (RK-PR) equation offers the best performance among cubic three-parameter density functionalities. A simple temperature dependence was developed and a straightforward parameterization procedure established. This simple - and optimized from pure compound data - three-parameter equation of state (3P-EoS) will allow in a later stage, by systematic study and comparison to other types of 3P-EoS, to find out what the actual possibilities and limitations of cubic EoS are in the modelling of phase equilibria for asymmetric systems. (c) 2005 Elsevier B.V. All rights reserved.

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Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.874 SNIP 0.998 CiteScore 1.99
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
We present solubility and diffusion data for the gases methane and carbon dioxide in the polymer poly(vinylidene fluoride). The polymer was cut from extruded piping intended for use in offshore oil and gas applications. Measurements were carried out using a purpose-built high-pressure microbalance. These properties were determined in the temperature range 80-120 degrees C and in the pressure range 50-150 bar for methane and 20-40 bar for carbon dioxide. In general, good agreement was obtained for similar measurements reported in the literature. Solubility follows a Henry’s law (linear) dependence with pressure. Diffusion coefficients for each of the gases in the polymer were also measured using the balance. Activation energies for diffusion and heats of solution for the two gases in the polymer were also determined. (C) 2004 Elsevier Ltd. All rights reserved.
Directs measurement of high temperature/high pressure solubility of methane and carbon dioxide in polyamide (PA-11) using a high-pressure microbalance

Experiments to determine the solubility of methane and carbon dioxide in PA-11 have been performed in the temperature range 50-90°C and the pressure ranges 50-150 bar for methane and 20-40 bar for carbon dioxide. In general, the results agree fairly well with previous experiments for similar polymers, as well as showing correct trends in terms of temperature and pressure. The solubility of the gases follows Henry's law-type behavior except for methane at very high pressures. Diffusivities were also measured for the same systems at the same conditions. While the diffusivities are subject to more uncertainty than the solubility measurements, the expected (Arrhenius) trends are observed. Agreement with other experimental data using different methods is also good.
Dynamic viscosity modeling of methane plus n-decane and methane plus toluene mixtures: Comparative study of some representative models

Viscosity measurements of well-defined mixtures are useful in order to evaluate existing viscosity models. Recently, an extensive experimental study of the viscosity at pressures up to 140 MPa has been carried out for the binary systems methane + n-decane and methane + toluene, between 293.15 and 373.15 K and for several methane compositions. Although very far from real petroleum fluids, these mixtures are interesting in order to study the potential of extending various models to the simulation of complex fluids with asymmetrical components (light/heavy hydrocarbon). These data (575 data points) have been discussed in the framework of recent representative models (hard sphere scheme, friction theory, and free volume model) and with mixing laws and two empirical models (particularly the LBC model which is commonly used in petroleum engineering, and the self-referencing model). This comparative study shows that the average absolute deviation of the models is between 3.8 and 49.8%, and the maximum deviation is between 11.6 and 78.4%, depending on the considered model.
Effect of asphaltenes on crude oil wax crystallization

The paper summarizes the experimental work done on asphaltene influenced wax crystallization. Three different asphaltenes (from stable oil, instable oil, and deposit) were mixed at several concentrations or dispersions into the waxy crude oil. These blends were evaluated by viscometry and yield stress measurement and compared with the original crude oil. A complex asphaltene–wax interaction as a function of asphaltene concentration and degree of asphaltene dispersion under dynamic and static condition was observed. The crystallization and the wax network strength was strongly dependent on the degree of asphaltene dispersion. The effect of asphaltenes on the wax appearance temperature (WAT) was examined by polarized light microscopy. The idea that the WAT is a function of asphaltene surface area was introduced and supported by experiment. It was observed that well-dispersed asphaltenes influence the wax crystallization at static condition more significantly than the more flocculated.

General information
Effect on molecular interactions of chemical alteration of petroleum asphaltenes. I

Asphaltenes are naturally occurring components of crude oil and have been the subject of many studies that have involved a variety of methods to determine their complex structure, their association in crude oil with resins, and their agglomeration phenomena. Yet, the molecular structures of asphaltenes have not been fully elucidated. It is especially important to characterize the polar functionalities of these fractions, because they participate in the intermolecular aggregation by means of hydrogen bonds. The chemical derivatization of asphaltenes has been used, in combination with suitable analysis techniques, to study the influence of these heteroatom groups on molecular interactions within these fractions. Methylation and trimethyl silylation of five asphaltenes from different sources was performed in the laboratory as an effort to understand the molecular interactions within these fractions. Experimental data from isothermal titration calorimetry has been used in assessing the role of polar hydrogen bonding functionalities in self-association of these complex molecules. Stability characteristics of these altered asphaltenes have further been studied by onset flocculation titration and compared with data for starting (unaltered) asphaltenes. Changes at the molecular level were also investigated by infrared and fluorescence spectroscopy and size exclusion chromatography. It was observed that the asphaltenes that were most susceptible to these reaction chemistries were also the stable asphaltenes in crude oil. It has been inferred that the stability of these asphaltenes in crude oil definitely can be related to the extent of intrinsic polarity.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Phase Equilibria and Separation Processes, Center for Energy Resources Engineering
Authors: Juyal, P. (Intern), Garcia, D. M. (Intern), Andersen, S. I. (Intern)
Pages: 1272-1281
Publication date: 2005
Conference: 5th International Conference on Petroleum Phase Behavior and Fouling, Banff, Canada, 13/06/2004 - 13/06/2004
Main Research Area: Technical/natural sciences

Publication information
Journal: Energy & Fuels
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BFI (2018): BFI-level 2
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Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.49
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 3.34
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 3.3
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 3.52
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 3.25
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
Experimental determination of solubility parameters of oils as a function of pressure
In this work, the solubility parameter of dead and live crude oils was measured at 303.15 K and up to 300 bar, using the internal pressure approach. An indirect technique was chosen, using thermal expansivities (determined from microcalorimetric measurements) and isothermal compressibilities (calculated from density measurements). This method was tested on seven pure compounds, and the deviation with literature data is <1 MPa$^{1/2}$. A method based on the refractive index was used to examine the validity of the results for the oils, and a deviation of <0.8 MPa$^{1/2}$ was observed. A modified solubility parameter was also calculated from two cubic equations of state and compared to experimental results. In this case, the deviations are larger (up to 6.5 MPa$^{1/2}$), whereas this approach gives accurate results for pure compounds. This might be due to the characterization procedure, because the volumes are measured and given as input. Therefore, a more appropriate characterization method should give better results.

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering, Technical University of Denmark
Authors: Verdier, S. C. R. (Intern), Duong, D. (Ekstern), Andersen, S. I. (Intern)
Pages: 1225-1229
Publication date: 2005
Conference: 5th International Conference on Petroleum Phase Behavior and Fouling, Banff, Canada, 13/06/2004 - 13/06/2004
Main Research Area: Technical/natural sciences

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Journal: Energy & Fuels
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Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.49
Experimental measurement and modeling of the distribution of solvent and ions between an aqueous phase and an ion exchange resin

The distribution of solutes and solvent between an aqueous solution of salt and an ion exchange resin has been measured at ambient temperature. The experiments have been performed for aqueous solutions of KNO₃, KCl, Ca(NO₃)₂ and CaCl₂ in the concentration range of 0-3N. The absorption has been measured for 3 gel type and 3 macroreticular resins with a degree of crosslinking varying from 10.5 to 18.5%. The experimental results have been modeled with the Extended UNIQUAC model combined with an elastic term taking the elastic properties of the resin structure into account. The model shows very good predictions with varying degree of crosslinking, and the deviations between model results and experimental data are all within the experimental error.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Christensen, S. G. (Intern), Thomsen, K. (Intern)
Pages: 247-260
Publication date: 2005
Main Research Area: Technical/natural sciences
Extension of the cubic-plus-association (CPA) equation of state to amines

The cubic-plus-association (CPA) equation of state has been extended to modeling mixtures containing amines. Special focus was given to primary and secondary amines, which are known to self-associate, thus forming hydrogen bonds in mixtures with alkanes. Pure-compound parameters have been determined from vapor pressure and liquid density data, but phase equilibrium data were also used as guidance for selecting the optimum sets among those which best represent the pure-compound properties. Diethylamine was modeled as a two-site molecule, whereas the two primary amines considered (methylamine, ethylamine) were modeled using both the two-site and three-site schemes. Both schemes perform overall equally well, when care is exercised in the parameter estimation, by giving more weight on the vapor pressures rather than the liquid densities. Thus, only results using the two-site scheme are shown. Excellent binary vapor-liquid equilibria have been obtained for amine + aliphatic hydrocarbons with a low value of the binary interaction parameter. Satisfactory results are obtained also for cross-associating systems with alcohols but less so with water, using, moreover, a rather high value of the interaction parameter.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Phase Equilibria and Separation Processes, Center for Energy Resources Engineering
Authors: Kaarsholm, M. K. (Intern), Derawi, S. (Intern), Michelsen, M. L. (Intern), Kontogeorgis, G. (Intern)
Pages: 4406-4413
Publication date: 2005
Main Research Area: Technical/natural sciences

Publication information
Journal: Industrial & Engineering Chemistry Research
Volume: 44
Issue number: 12
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Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.1 SJR 0.945 SNIP 1.139
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.949 SNIP 1.146 CiteScore 2.87
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.012 SNIP 1.292 CiteScore 2.85
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 0.982 SNIP 1.243 CiteScore 2.6
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.066 SNIP 1.338 CiteScore 2.56
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
High-pressure viscosity measurements for the ethanol plus toluene binary system

The viscosity of the ethanol + toluene binary system has been measured with a falling-body viscometer for seven compositions as well as for the pure ethanol in the temperature range from 293.15 to 353.15 K and up to 100 MPa with an experimental uncertainty of 2%. At 0.1 MPa the viscosity has been measured with a classical capillary viscometer (Ubbelohde) with an uncertainty of 1%. A total of 209 experimental measurements have been obtained for this binary system, which reveals a non-monotonic behavior of the viscosity as a function of the composition, with a minimum. The viscosity behavior of this binary system is interpreted as the result of changes in the free volume, and the breaking or weakening of hydrogen bonds. The excess activation energy for viscous flow of the mixtures is negative with a maximum absolute value of 335 J/(mol·K), indicating that this binary system is a very weakly interacting system showing a negative deviation from ideality. The viscosity of this binary system is represented by the Grunberg-Nissan and the Katti-Chaudhri mixing laws with an overall uncertainty of 12% and 8%, respectively. The viscosity of methanol (23 points) has also been measured in order to verify the calibration of the falling-body viscometer within the considered T, P range.

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Zeberg-Mikkelsen, C. K. (Intern), Baylaucq, A. (Ekstern), Watson, G. (Ekstern), Boned, C. (Ekstern)
Pages: 1289-1302
Publication date: 2005
Main Research Area: Technical/natural sciences
Internal pressure and solubility parameter as a function of pressure

The main goal of this work was to measure the solubility parameter of a complex mixture, such as a crude oil, especially as a function of pressure. Thus, its definition is explained, as well as the main approximations generally used in literature. Then, the internal pressure is investigated, since it is presented as an alternative of the solubility parameter. In this work, the assumption that internal pressure is a measure of the physical solubility parameter was made, i.e. representing the dispersion and polar forces. As for the pressure influence, it was seen that internal pressure reaches a maximum contrary to solubility parameter. An indirect method was chosen to estimate internal pressure, using thermal expansivities (determined by microcalorimetry) and isothermal compressibilities (determined by density measurements). The uncertainty is within 2% for the expansivity and 0.1% for the density. Five pure compounds (four hydrocarbons and I alcohol) were investigated at 303.15 K and up to 30 MPa, as well as a dead crude oil. The "physical" solubility parameter is slightly increasing with pressure (up to 0.8 MPa1/2 for cyclohexane) and, at 0.1 MPa, the difference with literature data is less than 1 MPa1/2 for hydrocarbons. On the contrary, the difference reaches 9 MPa1/2 for ethanol as expected, due to the presence of hydrogen bonding. A dead crude oil was also studied and its solubility parameter is within the expected range. Two cubic equations of states (Peng-Robinson and Soave-Redlich-Kwong) were able to approximate the "physical" solubility parameter of n-heptane (within 0.2 MPa1/2), providing that the volumes were measured and used as input. The Peng-Robinson equation gave somewhat better results.

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Verdier, S. C. R. (Intern), Andersen, S. I. (Intern)
Pages: 125-137
Publication date: 2005
Main Research Area: Technical/natural sciences

Publication information
Journal: Fluid Phase Equilibria
Volume: 231
Issue number: 2
ISSN (Print): 0378-3812
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 2.33 SJR 0.869 SNIP 1.155
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.874 SNIP 0.998 CiteScore 1.99
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 0.982 SNIP 1.248 CiteScore 2.28
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.007 SNIP 1.274 CiteScore 2.31
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.152 SNIP 1.286 CiteScore 2.31
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.034 SNIP 1.234 CiteScore 2.26
ISI indexed (2011): ISI indexed yes
Investigating Equations of State for Associating Fluids Using Spectroscopy

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: von Solms, N. (Intern), Kofod, J. L. (Ekstern), Jensen, L. (Ekstern), Passos, C. P. (Ekstern), Derawi, S. (Intern), Andersen, S. I. (Intern), Michelsen, M. L. (Intern), Kontogeorgis, G. (Intern)
Publication date: 2005
Event: Abstract from 21st European Symposium on Applied Thermodynamics, Jurata, Poland.
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 185204
Publication: Research - peer-review ∘ Conference abstract for conference – Annual report year: 2005

Investigating models for associating fluids using spectroscopy
Two equations of state (PC-SAFT and CPA) are used to predict the monomer fraction of pure associating fluids. The models each require five pure-component parameters usually obtained by fitting to experimental liquid density and vapor pressure data. Here we also incorporate monomer fractions measured using spectroscopy, resulting in models that better predict the monomer fraction (fraction of molecules not participating in hydrogen bonding), without sacrificing the accuracy of the liquid density and vapor pressure correlations. Thus, it is clear that monomer fraction prediction depends on the way the parameters were obtained. The selection of appropriate association schemes is also investigated using spectroscopic data. For pure water a four-site scheme is shown to be the most appropriate scheme. In the case of pure alcohols, a three-site scheme is best for methanol; two- or three-site schemes perform about equally for ethanol; for higher alcohols a two-site scheme is preferred. This is in accordance with steric arguments. Some difficulties in the interpretation of
spectroscopic data and their comparison with the predictions of association models are illustrated. Apparently anomalous
data from different sources are shown to be consistent if interpreted correctly.
Leaching of Nutrient Salts from Fly Ash from Biomass Combustion

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Department of Systems Biology, Department of Mechanical Engineering, Center for Energy Resources Engineering
Authors: Thomsen, K. (Intern), Vu, D. T. (Intern), Stenby, M. (Intern), Jensen, J. P. (Intern), Simonsen, P. S. (Intern), Sander, B. (Ekstern)
Publication date: 2005
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 188059
Publication: Research - peer-review › Poster – Annual report year: 2005

Modeling diffusion coefficients in binary mixtures of polar and non-polar compounds
The theory of transport coefficients in liquids, developed previously, is tested on a description of the diffusion coefficients in binary polar/non-polar mixtures, by applying advanced thermodynamic models. Comparison to a large set of experimental data shows good performance of the model. Only four temperature-independent parameters are required in order to describe the behavior of diffusion coefficients at different temperatures. The physical meaning of the parameters is analyzed. This makes it possible to reduce further their number to just two parameters for described mixtures with polar components and to only one parameter for mixtures consisting of non-polar components. A possibility of complete prediction of the parameters is discussed.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Phase Equilibria and Separation Processes, Center for Energy Resources Engineering
Authors: Medvedev, O. (Intern), Shapiro, A. (Intern)
Pages: 111-124
Publication date: 2005
Main Research Area: Technical/natural sciences

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Journal: Fluid Phase Equilibria
Volume: 236
Issue number: 1-2
ISSN (Print): 0378-3812
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 2.33 SJR 0.869 SNIP 1.155
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.874 SNIP 0.998 CiteScore 1.99
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 0.982 SNIP 1.248 CiteScore 2.28
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.007 SNIP 1.274 CiteScore 2.31
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.152 SNIP 1.286 CiteScore 2.31
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.034 SNIP 1.234 CiteScore 2.26
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 0.986 SNIP 1.317
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.133 SNIP 1.164
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.227 SNIP 1.09
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.031 SNIP 1.151
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.034 SNIP 1.245
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.009 SNIP 1.3
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 0.985 SNIP 1.349
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 1.193 SNIP 1.301
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 0.722 SNIP 1.101
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 0.966 SNIP 1.284
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 0.87 SNIP 0.898
Web of Science (2000): Indexed yes
Scopus rating (1999): SJR 0.938 SNIP 0.885
Original language: English
DOIs:
10.1016/j.fluid.2005.04.023
Modeling Electrolyte Solutions with the extended universal quasichemical (UNIQUAC) Model

The extended universal quasichemical (UNIQUAC) model is a thermodynamic model for solutions containing electrolytes and non-electrolytes. The model is a Gibbs excess function consisting of a Debye-Hückel term and a standard UNIQUAC term. The model only requires binary, ion specific interaction parameters. A unique choice of standard states makes the model able to reproduce solid-liquid, vapor-liquid, and liquid-liquid phase equilibria as well as thermal properties of electrolyte solutions using one set of parameters.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Thomsen, K. (Intern)
Pages: 531-542
Publication date: 2005
Main Research Area: Technical/natural sciences

Publication Information
Journal: Journal of Pure and Applied Chemistry
Volume: 77
Issue number: 3
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Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.45 SJR 0.972 SNIP 1.049
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.885 SNIP 0.853 CiteScore 2.09
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.066 SNIP 1.244 CiteScore 2.76
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.134 SNIP 1.145 CiteScore 2.72
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.347 SNIP 1.224 CiteScore 2.8
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.215 SNIP 1.058 CiteScore 2.56
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.987 SNIP 0.882
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.185 SNIP 0.988
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.103 SNIP 1.086
Scopus rating (2007): SJR 1.266 SNIP 1.059
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 0.722 SNIP 0.943
Scopus rating (2005): SJR 0.778 SNIP 0.995
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 0.595 SNIP 0.834
Modeling of aqueous electrolyte solutions with perturbed-chain statistical associated fluid theory

The vapor pressures and liquid densities of single-salt electrolyte solutions containing NaCl, LiCl, KCl, NaBr, LiBr, KBr, NaI, LiI, KI, Li2SO4, Na2SO4, and K2SO4 were modeled with an equation of state based on perturbed-chain statistical associated fluid theory (PC-SAFT). The PC-SAFT model was extended to charged compounds using a Debye-Huckel term for the electrostatic interactions. Two model parameters for each ion were fitted to experimental pVT and vapor-pressure data. The model is able to excellently reproduce the experimental data up to high salt molalities and even to predict vapor pressures in mixed-salt solutions.

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering, University of Dortmund
Authors: Cameretti, L. F. (Ekstern), Sadowski, G. (Ekstern), Mollerup, J. (Intern)
Pages: 3355-3362
Publication date: 2005
Main Research Area: Technical/natural sciences

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Volume: 44
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Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.1 SJR 0.945 SNIP 1.139
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.949 SNIP 1.146 CiteScore 2.87
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.012 SNIP 1.292 CiteScore 2.85
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 0.982 SNIP 1.243 CiteScore 2.6
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.066 SNIP 1.338 CiteScore 2.56
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.086 SNIP 1.24 CiteScore 2.58
Molecular dynamics simulations of the penetration lengths: application within the fluctuation theory for diffusion coefficients

Mutual diffusion in condensed phases is a theoretically and practically important subject of active research. One of the most rigorous and theoretically advanced approaches to the problem is a recently developed approach based on the concept of penetration lengths (Physica A 320 (2003) 211; Physica A 322 (2004) 151). In the current study, a fast molecular dynamics scheme has been developed to determine the values of the penetration lengths in Lennard-Jones binary systems. Results deduced from computations provide a new insight into the concept of penetration lengths. It is shown for four different binary liquid mixtures of non-polar components that computed penetration lengths, for various temperatures and compositions, are consistent with those deduced from experiments in the framework of the formalism of the fluctuation theory. Moreover, the mutual diffusion coefficients obtained from a coupled fluctuation theory and molecular dynamics scheme exhibit consistent trends and average deviations from experimental data around 10-20%. (c) 2004 Elsevier B.V. All rights reserved.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Phase Equilibria and Separation Processes, Center for Energy Resources Engineering
Authors: Galliero, G. (Ekstern), Medvedev, O. (Intern), Shapiro, A. (Intern)
Pages: 315-337
Publication date: 2005
Main Research Area: Technical/natural sciences

Publication information
Journal: Physica A: Statistical Mechanics and its Applications
Phase and viscosity behaviour of refrigerant-lubricant mixtures

The understanding of thermophysical properties and phase behaviour of refrigerant-lubricant oil mixtures is highly important for the optimal design of refrigeration and air-conditioning systems. Refrigerant lubricant mixtures, which are likely to have strong asymmetry, can show complex phase behaviour such as closed miscibility gaps, open miscibility gaps, liquid-liquid-vapour equilibrium, and even barotropic phenomena (density inversions). In fact, the type of phase behaviour that refrigerant-lubricant mixtures may show is linked to the transition between different types of phase diagrams, mainly as a function of the molecular asymmetry. This also has a profound effect in the mixture transport properties. Thus, in this work the general aspects of phase and viscosity behaviour linked to the type of asymmetry found in refrigerant-lubricant mixtures are discussed in the context of phase behaviour phenomenology. (c) 2004 Elsevier Ltd and IIR. All rights reserved.

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Cisneros, S. (Intern), Garcia, J. (Ekstern), Fernandez, J. (Ekstern), Monsalvo, M. A. (Intern)
Pages: 714-724
Publication date: 2005
Main Research Area: Technical/natural sciences

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Journal: International Journal of Refrigeration
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BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.06 SJR 1.344 SNIP 1.598
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.396 SNIP 1.537 CiteScore 2.44
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.667 SNIP 2.117 CiteScore 2.6
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.461 SNIP 1.979 CiteScore 2.25
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.426 SNIP 1.908 CiteScore 2.09
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.308 SNIP 2.129 CiteScore 2.2
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.372 SNIP 1.786
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.569 SNIP 1.954
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Precipitation Caused by CO2 Injection: Experiments and Modelling

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Publication date: 2005
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 186250
Publication: Research - peer-review › Journal article – Annual report year: 2005

Prediction and correlation of high-pressure gas solubility in polymers with simplified PC-SAFT
Using simplified PC-SAFT we have modeled gas solubilities at high temperatures and pressures for the gases methane and carbon dioxide in each of the three polymers high-density polyethylene (HDPE), nylon polyamide-11 (PA-11), and poly(vinylidene fluoride) (PVDF). In general the results are satisfactory, using in most cases a single, temperature-independent value of the binary interaction parameter. In the cases of methane in HDPE and PVDF, a temperature-dependent binary interaction parameter was required. New pure component polymer parameters for PA-11 and PVDF were obtained using a recently developed prediction scheme which does not rely on binary experimental data.

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: von Solms, N. (Intern), Michelsen, M. L. (Intern), Kontogeorgis, G. (Intern)
Pages: 3330-3335
Publication date: 2005
Main Research Area: Technical/natural sciences
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Journal: Industrial & Engineering Chemistry Research
Volume: 44
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BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Pressure parameters are added to the Extended UNIQUAC model presented by Thomsen and Rasmussen (1999). The improved model has been used for correlation and prediction of solid-liquid equilibrium (SLE) of scaling minerals (CaSO₄, CaSO₄·2H₂O, BaSO₄ and SrSO₄) at temperatures up to 300°C and pressures up to 1000 bar. The results show that the Extended UNIQUAC model, with the proposed pressure parameters, is able to represent binary, ternary and quaternary solubility data within the experimental accuracy in the temperature range from -20 to 300°C, and the pressure range from 1 to 1000 bar.
Process engineering versus product engineering - A case study on volatile organic compounds removal

Three solutions for removing the dangerous volatile organic compound (VOC) xylene from an industrial coating process are presented and compared. Two of them are based on classical process engineering principles, i.e., development of separation-cleaning methods such as incineration and adsorption. The last approach is somewhat different and is based on the so-called product engineering concept, i.e., in this case, a change of the formulation so that xylene is entirely eliminated from the process. It is shown that both the process and the product engineering approaches yield viable solutions to the problem-need specified in the beginning of the project, but producing a novel formulation (chemical product design) represents a method that results to a completely xylene-free process which is environmentally and economically more interesting than those generated via the more traditional process engineering approaches.

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering, Aveiro University
Authors: Coutinho, J. A. (Ekstern), Vilela, T. (Ekstern), Pereira, P. (Ekstern), Santos, M. M. M. (Ekstern), Kontogeorgis, G. (Intern)
Pages: 1-5
Publication date: 2005
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Publication information
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Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.79 SJR 0.813 SNIP 1.303
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.855 SNIP 1.449 CiteScore 2.7
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.027 SNIP 1.692 CiteScore 2.91
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.957 SNIP 1.668 CiteScore 2.56
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.933 SNIP 1.614 CiteScore 2.31
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Thin films of crude oil samples were prepared for atomic force microscopy (AFM) analysis on the gold substrate. Sample preparation involved evaporation during a long (24 h) but mild thermal exposure (80 °C). Fourier transform infrared (FTIR) microscopy (reflectance spectroscopy) was employed to determine the quality of the thin film surface, before the morphology characterization. The surface reflectance spectra were compared to direct transmittance FTIR of liquid oil samples. The two FTIR techniques showed different spectral characteristics related to oxygenated functionalities. This clearly indicated that the surface of the thin films of the oil samples prepared for AFM is oxidized. Oil samples of different origin show different degrees of oxidation seen by the development of carboxylic acid vibrations at 1750 cm⁻¹ as well as vibrations in the 1300−1100 cm⁻¹ region. The relative degree of oxidation state was compared to surface morphology data by AFM previously reported. The reported results emphasize the advantage of complementary techniques (AFM/FTIR microscopy) in the analysis of petroleum thin films that should be considered during analysis and interpretation of this type of data.
Recent applications of the cubic-plus-association (CPA) equation of state to industrially important systems

The cubic-plus-association equation of state (CPA EoS) has been extended to phase equilibria of industrially important binary mixtures of alcohol-hydrocarbon, alcohol/glycol-water systems and mixtures with organic acids. The ability of the model to predict different types of equilibria was tested. Very satisfactory VLE and SLE prediction is achieved for alcohol-
hydrocarbon systems, while the sensitivity of the LLE to the interaction parameter is demonstrated. It has been shown that CPA can perform VLE/LLE/SLE calculations in the case of alcohol-hydrocarbon binary systems with a single interaction parameter. Satisfactory SLE correlation of alcohol/glycol-water systems is achieved using a single interaction parameter over an extended temperature range. Moreover, satisfactory prediction was achieved for the multiphase equilibria of the mixture acetic acid-water-hexane based solely on binary interaction parameters. (c) 2004 Elsevier B.V. All rights reserved.
Rescaling of three-parameter equations of state: PC-SAFT and SPHCT

Two-parameter equations of state like PR or SRK predict a universal critical compressibility factor for pure compounds, being intrinsically unable to reasonably describe the PVT properties of different fluids and their asymmetric mixtures, which require at least three component specific parameters in the density dependence. In this paper, we have explored the capabilities of the Perturbed-Chain Statistical Associating Fluid Theory (PC-SAFT) and the Simplified Perturbed Hard Chain Theory (SPHCT) equations of state to represent pure compound properties. Original parameters published by their respective authors overestimate critical temperatures, which is detrimental for the study and design of supercritical separation processes. Therefore, we have investigated here the performance of rescaled parameters for each model, i.e., those matching the experimental critical temperature and pressure of pure compounds. The rescaling of the size and energetic parameters as implemented in recent works in the literature was found to provide poor results, and instead a simple procedure to obtain optimized rescaled parameters from only T, P_c and the acentric factor is proposed. These parameters show a regular behaviour for n-alkanes with PC-SAFT and their performance is tested in this work also for carbon dioxide, using the recent equations by Span and Wagner as reference data. The proposed parameters reproduce vapour pressures with the same accuracy of PC-SAFT original parameters but assure an exact representation of the experimental critical pressure and temperature. However, this is achieved at the expense of underestimated liquid densities, this limitation being common to different models and becoming more pronounced for larger molecules. (c) 2005 Published by Elsevier B.V.

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering, Planta Piloto de Ingenieria Quimica
Authors: Cismondi, M. (Intern), Brignole, E. A. (Ekstern), Mollerup, J. (Intern)
Pages: 108-121
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Main Research Area: Technical/natural sciences

Publication information
Journal: Fluid Phase Equilibria
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BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
Towards Asphaltenes Characterization by Simple Measurements

Viscosity measurements and correlations of binary mixtures: 1,1,1,2-tetrafluoroethane (HFC-134a)+tetraethylene glycol dimethylether (TEGDME)
This paper reports viscosity data for the binary system 1, 1, 1,2-tetrafluoroethane (HFC-134a), x(1), +tetraethylene glycol dimethylether (TEGDME), 1 - x(1). The measurements (200 data points) were obtained at various pressures (between 10 and 100 MPa) in the homogeneous liquid state from T= 293.15-373.15 K. The measurements have been carried out with a falling body viscometer for four molar fractions x(1) =(0.28, 0.44, 0.63 and 0.88). The density values of this system were interpolated from previous results obtained at the laboratory. All of the available viscosity data, including pure HFC-134a and pure TEGDME (both previously studied at the laboratory), have been correlated using several viscosity models (mixing rules, self-refrencing model, hard-sphere theory, friction theory and free volume model). The resulting models are presented and discussed in this work. (c) 2005 Elsevier B.V. All rights reserved.
Volumetric properties under pressure for the binary system ethanol plus toluene

The density of the asymmetrical binary system composed of ethanol and toluene has been measured under pressure using a vibrating tube densimeter. The measurements have been performed for nine different compositions including the pure compounds at eight temperatures in the range 283.15–353.15 K and ten isobars up to 45 MPa. The uncertainty in the measured densities is estimated to be 0.1 kg m\(^{-3}\). The measured data has been used to study the behavior and influence of temperature, pressure and composition on the isothermal compressibility, the isobaric thermal expansion, and the excess molar volume. At several temperatures the isobaric thermal expansion shows a non-monotonic behavior versus composition, whereas the excess molar volumes reveal a complex sigmoid behavior. These results have been interpreted as changes in the free-volume and as the formation and weakening of the molecular interactions. The VLE behavior of this binary system within the considered temperature range is represented satisfactorily by the perturbed-chain statistical association fluid theory (PC-SAFT) equation of state with a single interaction parameter, although no cross association between ethanol and toluene is taken into account. The densities of this binary system (pure compounds and mixtures) are satisfactorily predicted by PC-SAFT with an overall AAD of 0.8%, but the behavior of the excess molar volume is not described correctly.
Wax Precipitation Modeled with Many Mixed Solid Phases

The behavior of the Coutinho UNIQUAC model for solid wax phases has been examined. The model can produce as many mixed solid phases as the number of waxy components. In binary mixtures, the solid rich in the lighter component contains little of the heavier component but the second phase shows substantial amounts of the lighter component dissolved in the heavier solid. Calculations have been performed taking into account the recrystallization of the solid alkanes into a second solid form. The Coutinho UNIQUAC model has been used to describe the lower-temperature solid phases. The higher-temperature mixed solid phase has been assumed to be either an ideal solution or to be described by Coutinho's Wilson activity coefficient model. This procedure accounts for more of the known behavior of mixed n-alkane solids. Comparison is also made with results assuming that all of the solid phases, both high-temperature and low-temperature forms, are pure. Model calculations compare well with the data of Pauly et al. for C18 to C30 waxes precipitating from n-decane solutions. (C) 2004 American Institute of Chemical Engineers.

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Heidemann, R. A. (Ekstern), Madsen, J. (Ekstern), Stenby, E. H. (Intern), Andersen, S. I. (Intern)
Pages: 298-308
Publication date: 2005
Main Research Area: Technical/natural sciences

Publication information
Journal: A I Ch E Journal
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BFI (2017): BFI-level 2
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.11 SJR 1.034 SNIP 1.268
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.085 SNIP 1.417 CiteScore 3.03
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.07 SNIP 1.332 CiteScore 2.86
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.05 SNIP 1.364 CiteScore 2.59
Direct measurement of gas solubilities in polymers with a high-pressure microbalance

Solubility and diffusion data are presented for methane and carbon dioxide gases in high-density polyethylene. The polymer was cut from extruded piping intended for use in offshore oil and gas applications. The measurements were carried out with a high-pressure microbalance. The properties were determined from 25 to 50°C and from 50 to 150 bar for methane and from 20 to 40 bar for carbon dioxide. In general, a good agreement was obtained with similar measurements reported in the literature. The solubility followed Henry's law (linear) dependence with pressure, except at high pressures for methane, for which negative deviations from Henry's law behavior were observed. The diffusion coefficients for each of the gases in the polymer were also measured with the balance, although the uncertainty was greater than for the solubility measurements. (C) 2003 Wiley Periodicals, Inc. J Appl Polym Sci 91: 1476-1488, 2004.
Densities and solubilities of Glycylglycine and Glycyl-L-Alanine in Aqueous Electrolyte Solutions

Solubilities of glycylglycine and glycyl-L-alanine in aqueous electrolyte solutions containing 0-6 molal NaCl, 0-1 molal Na2SO4, and 0-1 molal (NH4)(2)SO4, have been determined experimentally at 298.15 K and atmospheric pressure. The solubility of glycylglycine and glycyl-L-alanine in pure water is 1.74 and 4.78 mol/kg of water, respectively. The solubility of glycylglycine in salt solutions of NaCl, Na2SO4, and (NH4)(2)SO4 show a moderate salting-in effect. The solubility of glycyl-L-alanine show a minor or no salting-in effect at low salt concentrations and a moderate salting-out effect at higher salt concentrations in NaCl and Na2SO4, and in (NH4)(2)SO4 the solubility is almost constant. The densities of the solutions have been determined experimentally, and the volume expansions by dissolving salt and dipeptide in water have been calculated. (C) 2003 Elsevier B.V. All rights reserved.

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Breil, M. P. (Intern), Mollerup, J. (Intern), Rudolph, E. S. J. (Ekstern), Ottens, M. (Ekstern), van der Wielen, L. A. M. (Ekstern)
Pages: 221-225
Publication date: 1 Feb 2004
Main Research Area: Technical/natural sciences

Publication information
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Issue number: 2
ISSN (Print): 0378-3812
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BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 2.33 SJR 0.869 SNIP 1.155
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.874 SNIP 0.998 CiteScore 1.99
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 0.982 SNIP 1.248 CiteScore 2.28
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.007 SNIP 1.274 CiteScore 2.31
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.152 SNIP 1.286 CiteScore 2.31
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
Analysis of Asphaltenes Subfractionated by N-Methyl-2-pyrrolidone

When petroleum asphaltenes are analyzed using size exclusion chromatography (SEC), it is desirable to use a mobile phase that allows elevated temperatures and suppresses effects that are not related to size. Recent developments in the analysis of tars and pitch have tried to use N-methyl-2-pyrrolidone (NMP) as a mobile phase. However, an NMP-insoluble asphaltene fraction of 9-53 wt % was observed for different petroleum n-heptane asphaltenes. Further analysis of the insoluble fraction surprisingly has shown that this fraction hardly exhibits any ultraviolet-visible light absorption or fluorescence. This result implies that a substantial fraction of asphaltenes will not be represented in a fluorescence spectrum. This finding may have great implications in the capacity of fluorescence spectroscopy to analyze asphaltenes.

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Ascanius, B. E. (Intern), Garcia, D. M. (Intern), Andersen, S. I. (Intern)
Pages: 1827-1831
Publication date: 2004
Main Research Area: Technical/natural sciences

Publication information
Journal: Energy & Fuels
Analytical Model for 1-D Gas Flooding: Splitting between Hydrodynamics and Thermodynamics

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Pires, A. (Ekstern), Bedrikovetsky, P. G. (Ekstern), Shapiro, A. (Intern)
A Novel Approach to Liquid-Liquid Equilibrium in Polymer Systems with Applications to Simplified PC-SAFT

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: von Solms, N. (Intern), Kouskoumvekaki, E. (Intern), Lindvig, T. (Ekstern), Michelsen, M. L. (Intern), Kontogeorgis, G. (Intern)
Pages: 87
Publication date: 2004
Main Research Area: Technical/natural sciences

Publication information
Journal: Fluid Phase Equilibria
Volume: 222-223
Issue number: 0
ISSN (Print): 0378-3812
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 2.33 SJR 0.869 SNIP 1.155
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.874 SNIP 0.998 CiteScore 1.99
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 0.982 SNIP 1.248 CiteScore 2.28
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.007 SNIP 1.274 CiteScore 2.31
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.152 SNIP 1.286 CiteScore 2.31
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.034 SNIP 1.234 CiteScore 2.26
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 0.986 SNIP 1.317
Web of Science (2010): Indexed yes
A Novel Method for Estimating Pure-Component Parameters for Polymers: Application to the PC-SAFT Equation of State

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Phase Equilibria and Separation Processes, Center for Energy Resources Engineering
Authors: Kouskoumvekaki, E. (Intern), von Solms, N. (Intern), Lindvig, T. (Intern), Michelsen, M. L. (Intern), Kontogeorgis, G. (Intern)
Pages: 2830-2838
Publication date: 2004
Main Research Area: Technical/natural sciences

Publication information
Journal: Industrial & Engineering Chemistry Research
Volume: 43
Issue number: 11
ISSN (Print): 0888-5885
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BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.1 SJR 0.945 SNIP 1.139
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.949 SNIP 1.146 CiteScore 2.87
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Application of Property Models in Chemical Product Design

**General information**

**State:** Published

**Organisations:** Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, Center for Phase Equilibria and Separation Processes, Center for Energy Resources Engineering

**Authors:** Gani, R. (Intern), Abildskov, J. (Ekstern), Kontogeorgis, G. (Intern)

**Number of pages:** 436

**Publication date:** 2004

**Host publication information**
Application of the CPA equation of state to organic acids

The CPA (Cubic-Plus-Association) equation of state has been extended to modeling of organic acids. We will focus in this work on formic, acetic, and propanoic acids due to their importance to the chemical and petrochemical industries. Organic acids, unlike many other associating compounds, have a strong tendency to dimerise in the vapor phase at normal condition resulting in strong non-ideal behavior, even at low pressures. Pure compound parameters have been determined from vapor pressure and liquid density data for the three acids. Among the three tested association schemes (one-site, two-site, and four-site), only the one-site association scheme describes satisfactorily the association in both the gas and the liquid phase. Second virial coefficients are predicted well with the proposed one-site model. Excellent binary VLE and acceptable LLE correlations have been obtained for acid + aliphatic hydrocarbons employing a low value of a binary interaction parameter. (c) 2004 Elsevier B.V. All rights reserved.
Application of the Perturbed Chain SAFT Equation of State to Complex Polymer Systems using Simplified Mixing Rules

General information
State: Published
Organisations: Department of Systems Biology, Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Kouskoumvekaki, I. (Intern), von Solms, N. (Intern), Michelsen, M. L. (Intern), Kontogeorgis, G. (Intern)
Pages: 71-78
Publication date: 2004
Main Research Area: Technical/natural sciences

Publication information
Journal: Fluid Phase Equilibria
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Web of Science (2017): Indexed yes
BDI (2016): BFI-level 2
Scopus rating (2016): CiteScore 2.33 SJR 0.869 SNIP 1.155
Web of Science (2016): Indexed yes

Original language: English
DOIs:
10.1016/jfluid.2004.08.021
Source: orbit
Source-ID: 186262
Publication: Research - peer-review › Journal article – Annual report year: 2004
Application of the Simplified PC-SAFT Equation of State to the Vapor Liquid Equilibria of Binary Mixtures of Polyamide 6 with Several Solvent

General information
State: Published
Organisations: Department of Systems Biology, Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Applied thermodynamics in chemical engineering in the 20th and 21st centuries

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Stenby, E. H. (Intern), Kontogeorgis, G. (Intern)
Number of pages: 234
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Host publication information
Title of host publication: BRIDGING from technology to society : DTU 1829-2004 - 175 år
Place of publication: Lyngby
Publisher: Technical University of Denmark (DTU)
Editors: Stubkjær, K., Kortenbach, T.
ISBN (Print): 9788799037803
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 209196
Publication: Research - peer-review › Journal article – Annual report year: 2004

Applying Association Theories to Polar Fluids

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: von Solms, N. (Intern), Michelsen, M. L. (Intern), Kontogeorgis, G. (Intern)
Pages: 1803-1806
Publication date: 2004
Main Research Area: Technical/natural sciences

Publication information
Journal: Industrial & Engineering Chemistry Research
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Ratings:
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BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.1 SJR 0.945 SNIP 1.139
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.949 SNIP 1.146 CiteScore 2.87
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Asphaltene self-association: Modeling and effect of fractionation with a polar solvent

The self-association of asphaltenes in toluene is believed to occur step-wise, rather than by the formation of micelles. A number of step-wise models have been used to fit the calorimetric titration of asphaltenes in dried toluene solutions, with excellent results. All the models are based on chemical reactions equivalent to the ones found in polymerization. The study shows that the choice of the average properties of asphaltenes, such as the molecular weight, is critical in the final value of the parameter of interest, namely the average heat of self-association ΔH(a). The low values of ΔH(a) obtained suggest that a fraction of asphaltenes is not active in the calorimetric experiments. Asphaltenes from Venezuela (LM1) and Mexico (KU) have been fractionated by precipitation with a mixture of acetone and toluene. It is considered that the most polar compounds are collected in the soluble fraction. A calorimetry study was performed on the two fractions, and the results show that the soluble fraction (SOL) has a much higher heat developed than the insoluble fraction (INS). This suggests again that a fraction of asphaltenes is not active in the calorimetric experiments, either because it does not self-associate or because the dilution effect is not strong enough to break the aggregates. Fluorescence and IR
spectroscopy experiments confirm there is self-association in INS fraction, leading to the conclusion that asphaltene aggregates are formed by bonds of different strengths. The stronger aggregates would be predominantly in INS fraction and would be inactive in the calorimetric experiments.
Barotropic Phenomena in Complex Phase Behaviour

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Cisneros, E. S. P. (Intern)
Pages: 2307-2313
Publication date: 2004
Main Research Area: Technical/natural sciences

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Journal: Physical Chemistry Chemical Physics
Volume: 6
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Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 4.06 SJR 1.678 SNIP 1.117
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.771 SNIP 1.244 CiteScore 4.45
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.772 SNIP 1.253 CiteScore 4.29
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.715 SNIP 1.216 CiteScore 4.05
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.916 SNIP 1.184 CiteScore 3.67
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.697 SNIP 1.203 CiteScore 3.6
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.802 SNIP 1.196
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 2.127 SNIP 1.369
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Carbon Dioxide and Hydrogen Sulfide Absorption Into Aqueous Solutions of Alkanolamines

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Kontogeorgis, G. (Intern), Coutsikos, P. (Ekstern)
Publication date: 2004

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 209182
Publication: Research - peer-review › Journal article – Annual report year: 2004

Chemical Product Design: A new challenge of applied thermodynamics

Chemical products involving specialty chemicals and microstructured materials are often multicomponent systems. A number of five to 20 molecules is not unusual, comprising a range of different chemical compounds e.g. polymers, surfactants, solid particles and water. Milk is an example of such a product involving both solid-liquid phases and (non-equilibrium) metastable states. Thus, many of these products are colloidal systems of different types, e.g. liquid-liquid emulsions, suspensions, powders, solid and liquid dispersions, aerosols and sprays. The physical chemistry (thermodynamics, stability) of such products is often as important as their manufacture, while a number of non-traditional manufacturing/ separation processes are of relevance, e.g. emulsification, foaming, gelation, granulation and crystallization. Today, serious gaps exist in our thermodynamic modelling abilities when we try to describe and understand chemical products with traditional thermodynamic models, typically applicable to problems of petrochemical industries. The purpose of this article is two-fold: first to present some current and future challenges in thermodynamic modelling towards chemical product design, and then to outline some specific examples from our research activities in the area of thermodynamics for chemical products. The examples cover rather diverse areas such as interrelation between thermodynamic and engineering properties in detergents (surfactants), paint thermodynamics and the development of models for gas solubility in elastomeric polymers.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Abildskov, J. (Ekstern), Kontogeorgis, G. (Intern)
Direct Measurement of Gas Solubilities in Polymers Using a High-Pressure Microbalance

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, The Danish Polymer Centre, Center for Energy Resources Engineering
Authors: von Solms, N. (Intern), Nielsen, J. (Ekstern), Hassager, O. (Intern), Rubin, A. (Ekstern), Dandekar, A. (Ekstern), Andersen, S. I. (Intern), Stenby, E. H. (Intern)
Pages: 1476
Publication date: 2004
Publication information
Journal: Journal of Applied Polymer Science
Volume: 91
ISSN (Print): 0021-8995
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.73 SJR 0.532 SNIP 0.724
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.574 SNIP 0.827 CiteScore 1.74
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.658 SNIP 0.964 CiteScore 1.76
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.628 SNIP 1.085 CiteScore 1.71
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.658 SNIP 1.081 CiteScore 1.57
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.601 SNIP 0.965 CiteScore 1.45
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.679 SNIP 0.909
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.697 SNIP 0.825
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.647 SNIP 0.822
Scopus rating (2007): SJR 0.678 SNIP 0.931
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 0.782 SNIP 1.145
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 0.779 SNIP 0.912
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 0.774 SNIP 0.962
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 0.816 SNIP 1.067
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 0.866 SNIP 1.084
Scopus rating (2001): SJR 0.964 SNIP 1.157
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 0.864 SNIP 1.157
Equations of State with Emphasis on Excess Gibbs Energy Mixing Rules

**General information**
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Epaminondas, V. C. (Ekstern), Coutsikos, P. (Ekstern), Kontogeorgis, G. (Intern)
Number of pages: 436
Publication date: 2004

**Host publication information**
Title of host publication: Computer Aided Property Estimation for Process and Product Design
Volume: PART II
Publisher: Elsevier
ISBN (Print): 978-0-444-51153-9
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 209325
Publication: Research - peer-review › Book chapter – Annual report year: 2004

Extended UNIQUAC Model for Correlation and Prediction of Vapor-Liquid-Liquid-Solid Equilibria in Aqueous Salt Systems Containing Non-Electrolytes. Part B. Alcohol (Ethanol, Propanols, Butanols) - Water-salt systems

The Extended UNIQUAC model for electrolyte solutions is an excess Gibbs energy function consisting of a Debye-Hückel term and a term corresponding to the UNIQUAC equation. For vapor-liquid equilibrium calculations, the fugacities of gas-phase components are calculated with the Soave-Redlich-Kwong equation of state. The model only requires binary, temperature-dependent interaction parameters. It has previously been used to describe the excess Gibbs energy for aqueous electrolyte mixtures and aqueous electrolyte systems containing methanol. It has been found to be an adequate model for representing solid-liquid-vapor equilibrium and thermal property data for strongly non-ideal systems. In this work, the model is extended to aqueous salt systems containing higher alcohols. The calculations are based on an extensive database consisting of salt solubility data, vapor liquid equilibrium data, and liquid-liquid equilibrium data for solvent mixtures and for mixed solvent-electrolyte systems.

The application of this model to represent the vapor-liquid-liquid-solid equilibria in aqueous systems containing various non-electrolytes (ethanol, 1-propanol, 2-propanol, 1-butanol, 2-butanol, 2-methyl 1-propanol, 2-methyl 2-propanol) and various ions (Na+, K+, NH4+, Cl-, NO3, SO42-, SO32-, HSO3-, CO32-, and HCO3-) shows the capability of the model to accurately represent the phase behavior of these kinds of systems. (C) 2004 Elsevier Ltd. All rights reserved.

**General information**
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Thomsen, K. (Intern), Iliuta, M. C. (Ekstern), Rasmussen, P. (Intern)
Pages: 3631-3647
Publication date: 2004
Main Research Area: Technical/natural sciences

**Publication information**
Journal: Chemical Engineering Science
Volume: 59
Issue number: 17
ISSN (Print): 0009-2509
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Liquid-liquid equilibria for binary and ternary polymer solutions with PC-SAFT

Two algorithms for evaluating liquid-liquid equilibria (LLE) for binary and ternary polymer solutions are presented. The binary algorithm provides the temperature versus concentration cloud-point curve at fixed pressure, whereas the ternary algorithm provides component 1 versus component 2 concentration coexistence curves at fixed pressure and temperature. The algorithms automatically trace the entire liquid-liquid coexistence curves in steps by adjusting the step size, generating initial estimates, and subsequently solving the phase-equilibrium problem by a second-order method. The algorithms are used for investigating the correlative and predictive capabilities of the thermodynamic model PC-SAFT. The investigation shows that the model correlates well experimental LLE data for binary as well as ternary systems but further predicts the behavior of the ternary systems with reasonably good accuracy, even by using interaction parameters obtained from binary vapor-liquid equilibrium data.
Modeling Diffusion Coefficients in Binary Mixtures

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Medvedev, O. (Intern), Shapiro, A. (Intern)
Pages: 13-22
Publication date: 2004
Main Research Area: Technical/natural sciences

Publication Information
Journal: Fluid Phase Equilibria
Modeling of multicomponent vapor-liquid equilibria for polymer-solvent systems

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering, National Centre for Scientific Research "Demokritos", Pennsylvania State University
Authors: Kontogeorgis, G. (Intern), Economou, I. (Ekstern), Michelsen, M. L. (Intern), Danner, R. (Ekstern), Lindvig, T. (Intern)
Pages: 11-20
Publication date: 2004
Main Research Area: Technical/natural sciences

Publication information
Journal: Fluid Phase Equilibria
Volume: 220
Issue number: 1
ISSN (Print): 0378-3812
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 2.33 SJR 0.869 SNIP 1.155
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.874 SNIP 0.998 CiteScore 1.99
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 0.982 SNIP 1.248 CiteScore 2.28
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.007 SNIP 1.274 CiteScore 2.31
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.152 SNIP 1.286 CiteScore 2.31
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.034 SNIP 1.234 CiteScore 2.26
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 0.986 SNIP 1.317
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.133 SNIP 1.164
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.227 SNIP 1.09
Modelling of salt activities in aqueous amino acid solutions II. The Kirkwood theory

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Breil, M. P. (Intern), Mollerup, J. (Intern)
Publication date: 2004

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 209175
Publication: Research › Report – Annual report year: 2004

Modelling of salt activities in aqueous amino acid solutions I. The UNIQUAC model

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Breil, M. P. (Intern), Mollerup, J. (Intern)
Publication date: 2004

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 209174
Publication: Research › Report – Annual report year: 2004

Models for Polymer Solutions

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Part II: Models for Properties

Part I: Introduction to Computer Aided Property Estimation

Part IV: Challenges and Opportunities
Prediction of Phase Equilibria and Thermodynamic Properties of Refrigerant/Oil Solutions

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Medvedev, O. (Intern), Zhelezny, P. (Intern), Zhelezny, V. P. (Ekstern)
Pages: 29-38
Publication date: 2004
Main Research Area: Technical/natural sciences

Publication Information
Journal: Fluid Phase Equilibria
Volume: 215
ISSN (Print): 0378-3812
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 2.33 SJR 0.869 SNIP 1.155
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.874 SNIP 0.998 CiteScore 1.99
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 0.982 SNIP 1.248 CiteScore 2.28
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.007 SNIP 1.274 CiteScore 2.31
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.152 SNIP 1.286 CiteScore 2.31
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.034 SNIP 1.234 CiteScore 2.26
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 0.986 SNIP 1.317
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.133 SNIP 1.164
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.227 SNIP 1.09
PVT characterization and viscosity modeling and prediction of crude oils

In previous works, the general, one-parameter friction theory (f-theory), models have been applied to the accurate viscosity modeling of reservoir fluids. As a base, the f-theory approach requires a compositional characterization procedure for the application of an equation of state (EOS), in most cases a cubic EOS, to the description of the oil phase properties. Normally, such a procedure provides a method for characterizing an oil into a number of compound groups along with the critical constants and parameters that are required by the EOS. Thus, in this work, a compositional characterization method based on an accurate description of the fluid mass distribution is presented. The characterization procedure accurately matches the fluid saturation pressure. Additionally, a Peneloux volume translation scheme, capable of accurately reproducing the fluid density above and below the saturation pressure, is also presented. The combination of the mass characterization scheme presented in this work and the f-theory, can also deliver accurate viscosity modeling results. Additionally, depending on how extensive the compositional characterization is, the approach presented in this work may also deliver accurate viscosity predictions. The modeling approach presented in this work can deliver accurate viscosity and density modeling and prediction results over wide ranges of reservoir conditions, including the compositional changes induced by recovery processes such as gas injection.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering, Center for Energy Resources Engineering
Authors: Cisneros, E. S. P. (Intern), Dalberg, A. (Ekstern), Stenby, E. H. (Intern)
Pages: 1309-1325
Publication date: 2004
Main Research Area: Technical/natural sciences

Publication information
Journal: Petroleum Science and Technology
Volume: 22
Issue number: 9&10
ISSN (Print): 1091-6466
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 0.285 SNIP 0.508 CiteScore 0.6
Representation of Volumetric Data of Electrolyte Solutions at Varying Concentrations and Temperatures

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Phase Equilibria and Separation Processes, Center for Energy Resources Engineering
Authors: Christensen, S. G. (Intern), Thomsen, K. (Intern)
Publication date: 2004

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 209193
Publication: Research - peer-review › Journal article – Annual report year: 2004
The influence of retention on the plate height in ion-exchange chromatography

The plate heights for the amino acid tyrosine (anion exchange) and the polypeptide aprotinin (cation exchange) were determined on a porous media (Resource 15) and a get filled media (HyperD 20) at salt concentrations ranging from weak to strong retention. At a constant velocity, measurements showed that the plate height increase with increasing retention, went through a maximum, and finally, decreased as the retention increased, i.e., when the salt concentration was lowered further. The band broadening of a chromatographic peak in the column was caused by the axial dispersion and mass transfer. In this article, the rate of mass transfer in the particles is described by three different rate mechanisms, pore diffusion, solid diffusion, and parallel diffusion. The van Deemter equation was used to model the data to determine the mass-transfer properties. The development of the plate height with increasing retention revealed a characteristic behavior for each rate mechanism. In the pore diffusion model, the plate height increased toward a constant value at strong retention, while the plate height in the solid diffusion model decreased, approaching a constant value at strong retention. In the parallel diffusion model, both pore and solid diffusion took place. Therefore, the parallel diffusion model coincides with the pore diffusion model at weak retention and with the solid diffusion model at strong retention, while a maximum is reached at intermediate retention, resulting in a bell-shaped curve. This behavior corresponds to the observed variation of the plate height at constant velocity. Neither the pore nor the solid diffusion model can describe the experimental data while a satisfactory fit was obtained using the parallel diffusion model.
Theoretical and experimental comparison of the Soret coefficient for water-methanol and water-ethanol binary mixtures

In multicomponent mixtures, a much richer variety of phenomena can occur than in simple (single-component) fluids. Natural convection in single-component fluids is due to buoyancy forces caused by temperature gradients. In multicomponent mixtures, buoyancy forces may also be caused by concentration gradients. Because natural convection, molecular diffusion, and thermal conduction have different relaxation time scales, a wide variety of resulting convective motions and heat, and mass distributions may occur. In some fluid mixtures such as water-ethanol systems, for instance, ethanol diffuses much more slowly than heat, and because of this difference in time scales oscillatory convection might occur. In a multicomponent mixture, the total molar flux consists of two parts: the convective molar flux and the diffusive molar flux (resulting from the difference between the component, velocity and the bulk velocity). The diffusion molar flux of a component depends, not only, on its own mole fraction gradient (Fickian diffusion), but also on the gradient of all the components present in the mixture (cross-molecular diffusion). The diffusion flux depends also on the pressure gradient (pressure diffusion; the so-called -gravitational effect) and temperature gradient (thermal diffusion; the so-called Soret effect). Firoozabadi's thermal diffusion model was applied to calculate the Soret coefficient, as well as the thermal diffusion coefficient and molecular diffusion coefficient for methanol-water and ethanol-water mixtures at 310.65 K temperature and 1 bar pressure with 10% water mass fraction. The results were compared with experimental data (J.K. Platten. in Proceedings of the 5th, International Meeting on Thermodiffusion, (IMTS); Lyngby Aug. 2002 Philos. Mag. 83. Nos. 17-18 (2003)), as well as theoretical predictions with other models. A better agreement with the experimental data using the Firoozabadi model was achieved.
Thermodynamics of Electrolyte Systems of Industry

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Thomsen, K. (Intern)
Pages: 219-229
Three-phase Compositional Streamline Simulation and Its Application to WAG

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Yan, W. (Intern), Michelsen, M. L. (Intern), Stenby, E. H. (Intern), Berenblyum, R. (Intern), Shapiro, A. (Intern)
Number of pages: 11
Publication date: 2004
Event: Paper presented at SPE/DOE Symposium on Improved Oil Recovery, Tulsa, Oklahoma
Main Research Area: Technical/natural sciences
DOIs: 10.2118/89440-MS
Source: orbit
Source-ID: 262146
Publication: Research - peer-review › Paper – Annual report year: 2004

Upgrade of a Raman Spectrometer

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Hansen, S. B. (Ekstern), Berg, R. W. (Ekstern), Stenby, E. H. (Intern)
Pages: 385-397
Publication date: 2004
Main Research Area: Technical/natural sciences
Publication information
Journal: Applied Spectroscopy Reviews
Volume: 39
Issue number: 3
ISSN (Print): 0570-4928
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 4.82 SJR 0.937 SNIP 2.199
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.928 SNIP 1.892 CiteScore 4.27
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.199 SNIP 1.947 CiteScore 4.36
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.78 SNIP 1.405 CiteScore 3.37
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.973 SNIP 1.731 CiteScore 3.1
Van der Waals-based Cubic Equations of State for Asymmetric Systems using a Simple Mixing Rule

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Kontogeorgis, G. (Intern), Coutsikos, P. (Ekstern)
Publication date: 2004

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 188700
Publication: Research - peer-review › Report – Annual report year: 2004

Computational and Physical Performance of a Modified PC-SAFT Equation of State for Highly Asymmetric and Associating Mixtures

Two modifications to perturbed-chain statistical associating fluid theory are proposed which simplify the calculation of phase-equilibrium properties for nonassociating and associating systems, polymers, and simple molecules without loss of accuracy. A simple linear extrapolation scheme is proposed to obtain parameters for linear alkanes up to polyethylene. It is shown that computing times are greatly reduced using these modifications and compare favorably with traditional equations of state for nonassociating and associating systems.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: von Solms, N. (Intern), Michelsen, M. L. (Intern), Kontogeorgis, G. (Intern)
Pages: 1098-1105
Publication date: 5 Mar 2003
A Corresponding States Model for the Estimation of Thermophysical Properties of Asymmetric Mixtures

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Queimada, A. J. (Ekstern), Marrucho, I. M. (Ekstern), Stenby, E. H. (Intern), Coutinho, J. A. (Ekstern)
Publication date: 2003
Event:
Main Research Area: Technical/natural sciences
Source-ID: 138313
Publication: Research - peer-review › Journal article – Annual report year: 2003

AFM Characterization of Organic Deposits on Metal Substrates from Mexican Crude Oils

General information
State: Published
Organisations: Center for Energy Resources Engineering
Authors: Batina, N. (Ekstern), Manzano-Martinez, J. C. (Ekstern), Andersen, S. I. (Ekstern), Lira-Galeana, C. (Ekstern)
Pages: 532-542
Publication date: 2003
Main Research Area: Technical/natural sciences
Source-ID: 41110
Publication: Research › Poster – Annual report year: 2003
Analytical Integral Equation Theory for a Restricted Primitive Model of Polyelectrolytes and Counterions within the Mean Spherical Approximation. 2. Radial Distribution Functions

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: von Solms, N. (Intern), Chiew, Y. (Ekstern)
Pages: 4321
Publication date: 2003
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Chemical Physics
Volume: 118
ISSN (Print): 0021-9606
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 2.13 SJR 1.073 SNIP 0.755
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.953 SNIP 0.767 CiteScore 1.98
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.386 SNIP 0.989 CiteScore 2.54
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.532 SNIP 1.17 CiteScore 2.95
A new Corresponding States model for the estimation of thermophysical properties of long chain n-alkanes

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Queimada, A. J. (Ekstern), Stenby, E. H. (Intern), Marrucho, I. M. (Ekstern), Coutinho, J. A. (Ekstern)
Pages: 303-314
Publication date: 2003
Main Research Area: Technical/natural sciences

Publication information
Journal: Fluid Phase Equilibria
Volume: 212
Issue number: 1
ISSN (Print): 0378-3812
Ratings:
Application of the CPA equation of state to glycol/hydrocarbons liquid-liquid equilibria

The Cubic Plus Association (CPA) equation of state is a thermodynamic model, which combines the well-known cubic SRK (Soave-Redlich-Kwong) equation of state and the association term proposed by Wertheim, typically employed in models like SAFT (statistical associating fluid theory). CPA has been shown in the past to be a successful model for phase equilibria calculations for systems containing water, hydrocarbons and alcohols. In this work, CPA is applied for the first time to liquid-liquid equilibria (LLE) for systems containing glycols and hydrocarbons. It is shown that excellent correlation is achieved with solely a single interaction parameter per binary system. The correlation procedure as well as the nature of the experimental data play a crucial role in the parameter estimation and they are thus extensively discussed. (C) 2003 Elsevier Science B.V. All rights reserved.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Derawi, S. (Intern), Michelsen, M. L. (Intern), Kontogeorgis, G. (Intern), Stenby, E. H. (Intern)
Pages: 163-184
Publication date: 2003
Main Research Area: Technical/natural sciences

Publication information
Journal: Fluid Phase Equilibria
Volume: 209
Issue number: 2
ISSN (Print): 0378-3812
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2016): CiteScore 2.33 SJR 0.869 SNIP 1.155
Web of Science (2016): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 0.982 SNIP 1.248 CiteScore 2.28
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.007 SNIP 1.274 CiteScore 2.31
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.152 SNIP 1.286 CiteScore 2.31
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.034 SNIP 1.234 CiteScore 2.26
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 0.986 SNIP 1.317
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.133 SNIP 1.164
Web of Science (2009): Indexed yes
Application of the CPA equation of state to industrially important systems

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Derawi, S. (Intern), Michelsen, M. L. (Intern), Kontogeorgis, G. (Intern), Stenby, E. H. (Intern)
Publication date: 2003
Event: Poster session presented at 15 Years of the SAFT Equation, Barcelona, Spain.
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 138311
Publication: Research › Poster – Annual report year: 2003

Application of the CPA Equation of State to Industrially Important Systems

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Derawi, S. O. (Ekstern), Michelsen, M. L. (Intern), Kontogeorgis, G. (Intern), Stenby, E. H. (Intern)
Publication date: 2003
Event: Poster session presented at 20th European Symposium on Applied Thermodynamics, Lahnstein, Germany.
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 209197
Publication: Research › Poster – Annual report year: 2003

Applications of Association Models to problems of the Oil, Chemical and Polymer Industries

General information
State: Published
A Simplified PC-SAFT Equation of State: Multicomponent Liquid-Liquid Equilibrium in Polymer and Associating Systems

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: von Solms, N. (Intern), Lindvig, T. (Intern), Kouskoumvekaki, E. (Ekstern), Michelsen, M. L. (Intern), Kontogeorgis, G. (Intern)
Pages: 379-382
Publication date: 2003
Event: Poster session presented at 20th European Symposium on Applied Thermodynamics, Lahnstein, Germany.
Main Research Area: Technical/natural sciences
Source-ID: 41116
Publication: Research › Poster – Annual report year: 2003
Chemical product engineering of antifouling paints using mathematical modeling

General information
State: Published
Organisations: CHEC Research Centre, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Kiil, S. (Intern)
Publication date: 2003

Host publication information
Title of host publication: 7th International Conference on Chemical Engineering, Granada
Main Research Area: Technical/natural sciences
Conference: 7th International Conference on Chemical Engineering, Granada, Spain, 01/01/2003
Source: orbit
Source-ID: 41242
Publication: Research › Conference abstract in proceedings – Annual report year: 2003

Comparative Study of Viscosity Models on the Ternary System Methylcyclohexane + cis-Decalin + 2,2,4,4,6,8,8-Heptamethylnonane up to 100 MPa

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Zeberg-Mikkelsen, C. K. (Intern), Baylaucq, A. (Ekstern), Barrouhou, M. (Ekstern), Cisneros, S. (Intern)
Publication date: 2003
Event: Poster session presented at Symposium on Thermophysical Properties, Boulder, United States.
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 41098
Publication: Research › Poster – Annual report year: 2003

Comparisons Between Asphaltenes from the Dead and Live-Oil Samples of the Same Crude Oils
Asphaltenes precipitated from pressure-preserve bottomhole oil samples have been obtained for three oils at different pressures, using a bulk high-pressure filtration apparatus. The precipitates captured on the filter were recovered, the asphaltenes defined by the n-heptane insolubility were extracted and analyzed. These pressure-driven asphaltenes found on the filter were found to make up in the range between 50 and 100 ppm of the whole crude oil. Opening of the cell did not reveal asphaltenes retained due to wall adhesion. Size exclusion chromatography tests performed on both the live-oil-derived asphaltenes and the standard asphaltenes as precipitated by atmospheric titration on the same crude oil, revealed that the live-oil asphaltenes had apparent smaller hydrodynamic volume and narrower distributions than the standard asphaltenes for two oils. Further FTIR tests also showed large differences between standard asphaltenes and the asphaltenes obtained at high pressure filter. The latter appeared to contain more functional groups and be less saturated. Implication of these structural differences on precipitation modeling is discussed.

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Aquino-Olivos, M. (Ekstern), Andersen, S. I. (Intern), Lira-Galeana, C. (Ekstern)
Pages: 1017-1041
Publication date: 2003
Main Research Area: Technical/natural sciences
Publication information
Journal: Petroleum Science and Technology
Volume: 21
Issue number: 5
ISSN (Print): 1091-6466
Ratings:
Determination of isobaric thermal expansivity of organic compounds from 0.1 to 30 MPa at 30 degrees C with an isothermal pressure scanning microcalorimeter

This paper describes a simple high-pressure mercury-free microcalorimetric technique that enables the compression of a fluid from 0.1 to 30 MPa. Thermal expansivities of several compounds were calculated (n-hexane, cyclohexane, heptane, and toluene) with the pressure. scanning transitiometry method at 30 degreesC +/- 0.03 degreesC as a function of pressure and compared to the data found in the literature. The results are quite close to the literature values (4.2% at the very worst), and the uncertainty has been evaluated at 2%. A Tait equation, fitted from experimental density data, was also used to test the results of this work. The difference is between -5.9% and 3.2%.
General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Verdier, S. C. R. (Intern), Andersen, S. I. (Intern)
Pages: 892-897
Publication date: 2003
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Chemical and Engineering Data
Volume: 48
Issue number: 4
ISSN (Print): 0021-9568
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.29 SJR 0.88 SNIP 1.097
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.868 SNIP 0.966 CiteScore 1.96
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.021 SNIP 1.208 CiteScore 2.22
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.135 SNIP 1.199 CiteScore 2.17
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.141 SNIP 1.103 CiteScore 2.01
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.862 SNIP 0.988 CiteScore 1.8
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.054 SNIP 1.299
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.313 SNIP 1.037
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.505 SNIP 1.186
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.263 SNIP 1.254
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.146 SNIP 1.33
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.155 SNIP 1.342
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 0.897 SNIP 1.205
Scopus rating (2003): SJR 1.054 SNIP 1.157
Determination of the Pseudocritical Parameters for Refrigerant/Oil Solutions

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Zhelezny, P. (Intern), Zhelezny, V. P. (Ekstern), Scripov, P. (Ekstern)
Pages: 285-302
Publication date: 2003
Main Research Area: Technical/natural sciences

Publication information
Journal: Fluid Phase Equilibria
Volume: 212
Issue number: 0
ISSN (Print): 0378-3812
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 2.33 SJR 0.869 SNIP 1.155
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.874 SNIP 0.998 CiteScore 1.99
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 0.982 SNIP 1.248 CiteScore 2.28
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.007 SNIP 1.274 CiteScore 2.31
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.152 SNIP 1.286 CiteScore 2.31
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.034 SNIP 1.234 CiteScore 2.26
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 0.986 SNIP 1.317
Evaluation of diffusion coefficients in multicomponent mixtures by means of the fluctuation theory

We derive general expressions for diffusion coefficients in multicomponent non-ideal gas or liquid mixtures. The derivation is based on the general statistical theory of fluctuations around an equilibrium state. The matrix of diffusion coefficients is expressed in terms of the equilibrium thermodynamic characteristics of the mixture (such as molar densities and internal energy), as well as in terms of the newly introduced parameters, the penetration lengths. This result serves to reduce the problem of determining the diffusion coefficients to a smaller number of physically meaningful characteristics. We demonstrate on several examples that the developed theory is in agreement with the established experimental facts and dependencies for the diffusion coefficients. (C) 2002 Elsevier Science B.V. All rights reserved.
Evaluation of the Thermodynamic Models for the Thermal Diffusion Factor

Over the years, several thermodynamic models for the thermal diffusion factors for binary mixtures have been proposed. The goal of this paper is to test some of these models in combination with different equations of state. We tested the following models: those proposed by Rutherford and Drickamer in 1954, by Dougherty and Drickamer in 1955, by Haase in 1969, by Kempers in 1989 and 2002, and by Shucla and Firoozabadi in 1998. The calculated values of thermal diffusion factors were compared with a few sets of experimental data for hydrocarbon mixtures. For calculation of the partial molar properties we applied different thermodynamic models, such as the Soave-Redlich-Kwong and the Peng-Robinson equations of state. The necessity to try different thermo-dynamic models is caused by the high sensitivity of the thermal diffusion factors to the values of the partial molar properties. Two different corrections for the determination of the partial molar volumes have been implemented; the Peneloux correction and the correction based on the principle of corresponding states.

General information
State: Published
Extension of the cubic-plus-association equation of state to glycol-water cross-associating systems

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Derawi, S. (Intern), Michelsen, M. L. (Intern), Kontogeorgis, G. (Intern), Stenby, E. H. (Intern)
Pages: 1470-1477
Publication date: 2003
Main Research Area: Technical/natural sciences

Publication information
Journal: Industrial & Engineering Chemistry Research
Volume: 42
Issue number: 7
ISSN (Print): 0888-5885
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.1 SJR 0.945 SNIP 1.139
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.949 SNIP 1.146 CiteScore 2.87
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.012 SNIP 1.292 CiteScore 2.85
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 0.982 SNIP 1.243 CiteScore 2.6
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.066 SNIP 1.338 CiteScore 2.56
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.086 SNIP 1.24 CiteScore 2.58
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.047 SNIP 1.165
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.002 SNIP 1.164
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 1.142 SNIP 1.267
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.105 SNIP 1.239
Web of Science (2007): Indexed yes
Friction Theory Prediction of Crude Oil Viscosity at Reservoir Conditions Based on Dead Oil Properties

The general one-parameter friction theory (f-theory) models have been further extended to the prediction of the viscosity of real "live" reservoir fluids based on viscosity measurements of the "dead" oil and the compositional information of the live fluid. This work represents the viscosity of real fluids by a simple one-parameter tuning of a linear equation derived from a general one-parameter f-theory model. Further, this is achieved using simple cubic equations of state (EOS), such as the Peng-Robinson (PR) EOS or the Soave-Redlich-Kwong (SRK) EOS, which are commonly used within the oil industry. In the absence of compositional information, this work also presents a simple characterization procedure which is based on compositional information of an oil sample. This procedure provides a method for characterizing an oil into a number of compound groups along with the critical constants and parameters that are required by an EOS. The resulting EOS characterized fluid correctly reproduces properties such as the saturation pressure and the liquid phase density, from reservoir conditions to low pressure conditions. The viscosity modeling approach along with the characterization method presented in this work provide a complete self-consistent procedure for the viscosity and density modeling of reservoir fluids. (C) 2003 Elsevier B.V. All rights reserved.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Phase Equilibria and Separation Processes, Center for Energy Resources Engineering
Authors: Cisneros, S. (Intern), Zeberg-Mikkelsen, C. K. (Intern), Stenby, E. H. (Intern)
Pages: 233-243
Publication date: 2003
Main Research Area: Technical/natural sciences

Publication information
Journal: Fluid Phase Equilibria
Volume: 212
Issue number: 1-2
ISSN (Print): 0378-3812
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 2.33 SJR 0.869 SNIP 1.155
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Generalized Relation Between Surface Tension and Viscosity: a Study on Pure and Mixed n-Alkanes

General Information
State: Published
Measurement and Modeling of Surface Tensions of Asymmetric Systems: Heptane, Eicosane, Docosane, Tetracosane and their Mixtures

To extend the surface tension database for heavy or asymmetric n-alkane mixtures, measurements were performed using the Wilhelmy plate method. Measured systems included the binary mixtures heptane + eicosane, heptane + docosane and heptane + tetracosane and the ternary mixture heptane + eicosane + tetracosane at temperatures from 313.15 K (or above the melting point of the mixture) up to 343.15 K. All the measurements were performed at atmospheric pressure.

Using these data, along with data previously measured by us and collected from the literature, a recently proposed corresponding states model was assessed. It is shown that using a new generalized combining rule for the critical temperature, the data can be described with deviations of about 1% that is within the experimental uncertainty of the measurements. (C) 2003 Elsevier B.V. All rights reserved.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Queimada, A. (Intern), Silva, F. A. E. (Ekstern), Caco, A. I. (Ekstern), Marrucho, I. M. (Ekstern), Coutinho, J. (Intern)
Pages: 211-221
Publication date: 2003
Main Research Area: Technical/natural sciences
Publication information
Journal: Fluid Phase Equilibria
Volume: 214
Issue number: 2
ISSN (Print): 0378-3812
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 2.33 SJR 0.869 SNIP 1.155
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.874 SNIP 0.998 CiteScore 1.99
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 0.982 SNIP 1.248 CiteScore 2.28
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.007 SNIP 1.274 CiteScore 2.31
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.152 SNIP 1.286 CiteScore 2.31
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
Modeling of the water-hydrocarbon interface: Coupling the CPA EoS with the gradient theory

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Queimada, A. J. (Ekstern), Marrucho, I. M. (Ekstern), Stenby, E. H. (Intern), Kontogeorgis, G. (Intern), Miqueu, C. (Ekstern), Coutinho, J. A. (Ekstern)
Pages: 391-394
Publication date: 2003

Host publication information
Title of host publication: ESAT 2003, Germany
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 41365
Publication: Research › Conference abstract in proceedings – Annual report year: 2003
 Modeling of Vapor-Liquid Equilibria in the manufacturing Process of Nylon-6 with the modified PC-SAFT Equation of State

General information
State: Published
Organisations: Center for Biological Sequence Analysis, Department of Systems Biology, Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Kouskoumvekaki, I. (Intern), Krooshof, G. (Ekstern), Michelsen, M. L. (Intern), Kontogeorgis, G. (Intern)
Pages: 345-348
Publication date: 2003

Host publication information
Title of host publication: ESAT 2003
Main Research Area: Technical/natural sciences
Conference: 20th European Symposium on Applied Thermodynamics, Lahnstein, Germany, 08/10/2003 - 08/10/2003
Source: orbit
Source-ID: 209195
Publication: Research - peer-review › Article in proceedings – Annual report year: 2003

Modeling of Vapor-Liquid-Solid Equilibria in Acidic Aqueous Solutions
The phase behavior (vapor - liquid equilibria (VLE) and solid - liquid equilibria (SLE)) and thermal properties of aqueous solutions of ions like (K+, Na+, NH4+, Ca2+, Cl-) in the presence of phosphoric acid (H3PO4, H2PO4-, HPO42- ) and nitric acid (HNO3, NO3-) are described by means of the Extended UNIQUAC model. Model parameters are evaluated on the basis of more than 2000 experimental data points. There is good agreement between calculated and experimental data points. The model parameters are valid in the temperature range from -18°C to +122°C and in the concentration range up to 12 molal for the acids HNO3 and H3PO4.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Christensen, S. G. (Ekstern), Thomsen, K. (Intern)
Pages: 4260-4268
Publication date: 2003
Main Research Area: Technical/natural sciences

Publication information
Journal: Industrial & Engineering Chemistry Research
Volume: 42
Issue number: 18
ISSN (Print): 0888-5885
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.1 SJR 0.945 SNIP 1.139
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.949 SNIP 1.146 CiteScore 2.87
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.012 SNIP 1.292 CiteScore 2.85
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 0.982 SNIP 1.243 CiteScore 2.6
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.066 SNIP 1.338 CiteScore 2.56
ISI indexed (2012): ISI indexed yes
Modelling of Activity and Solubility of Amino Acids in Salt Solutions

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Breil, M. P. (Intern), Mollerup, J. (Intern)
Publication date: 2003
Event: Poster session presented at 20th European Symposium on Applied Thermodynamics, Lahnstein, Germany.
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 41094
Publication: Research - peer-review › Journal article – Annual report year: 2003

Modelling of multicomponent vapor-liquid equilibria for polymer-solvent systems

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering, Institute of Physical Chemistry, Pennsylvania State University
Modelling of the Adsorptive Properties of Whey Proteins on Anion Exchangers

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Phase Equilibria and Separation Processes, Center for Energy Resources Engineering
Authors: Frederiksen, S. S. (Intern), Pedersen, L. (Intern), Mollerup, J. (Intern)
Pages: 101-104
Publication date: 2003

Host publication information
Title of host publication: ESAT 2003
Main Research Area: Technical/natural sciences
Conference: 20th European Symposium on Applied Thermodynamics, Lahnstein, Germany, 08/10/2003 - 08/10/2003
Source: orbit
Source-ID: 209320
Publication: Research - peer-review › Article in proceedings – Annual report year: 2003

Molecular Size of Asphaltene Fractions Obtained from Residuum Hydrotreatment

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Buch, L. (Ekstern), Groenzin, H. (Ekstern), Buenrostro-Gonzalez, E. (Ekstern), Andersen, S. I. (Intern), Lira-Galeana, C. (Ekstern), Mullins, O. C. (Ekstern)
Pages: 1075-1084
Publication date: 2003
Main Research Area: Technical/natural sciences

Publication information
Journal: Fuel
Volume: 82
Issue number: 0
Original language: English
Source: orbit
Source-ID: 41229
Publication: Research - peer-review › Journal article – Annual report year: 2003

Phase Behaviour of Refrigerant-Lubricant Mixtures

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Quiñones-Cisneros, S. E. (Ekstern), Monsalvo, M. A. (Intern), Garcia, J. (Ekstern), Fernández, J. (Ekstern)
Pages: 223-226
Publication date: 2003

Host publication information
Phase Envelope Calculations for Hydrocarbon-Water Mixtures

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering, Calsep A/S
Authors: Lindeloff, N. (Ekstern), Michelsen, M. L. (Intern)
Pages: 298-303
Publication date: 2003
Main Research Area: Technical/natural sciences

Publication information
Journal: SPE Journal 77770
Volume: 8
Issue number: 3
Original language: English
Source: orbit
Source-ID: 41158
Publication: Research - peer-review › Journal article – Annual report year: 2003

Short Course on PC-SAFT

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: von Solms, N. (Intern)
Publication date: 2003

Publication information
Publisher: Internal Report
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 209324
Publication: Research - peer-review › Report – Annual report year: 2003

Supercritical Fluid Extraction of a-Methylene-g-Butyrolactone from Alstroemeria: Optimization by Statistical Experimental Design

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Hutchenson, K. W. (Ekstern), Jensen, O. F. (Ekstern), Kao, C. P. (Ekstern), Stenby, E. H. (Intern)
Publication date: 2003

Host publication information
Title of host publication: Proceedings of the 6th International Symposium on Supercritical Fluids
Main Research Area: Technical/natural sciences
Conference: International Symposium on Supercritical Fluids, Versailles, France, 01/01/2003
Source: orbit
Source-ID: 41095
Publication: Research › Conference abstract in proceedings – Annual report year: 2003
Verifying reciprocal relations for experimental diffusion coefficients in multicomponent mixtures

The goal of the present study is to verify the agreement of the available data on diffusion in ternary mixtures with the theoretical requirement of linear non-equilibrium thermodynamics consisting in symmetry of the matrix of the phenomenological coefficients. A common set of measured diffusion coefficients for a three-component mixture consists of four Fickian diffusion coefficients, each being reported separately. However, the Onsager theory predicts the existence of only three independent coefficients, as one of them disappears due to the symmetry requirement. Re-calculation of the Fickian diffusion coefficients into Onsager coefficients for a non-ideal mixture involves derivatives of the chemical potentials and, thus, should be based on a certain thermodynamic model (cubic equation of state (EoS), an activity coefficient model, etc.). Transformation of the Fickian diffusion coefficients into Onsager coefficients and a subsequent symmetry check make it possible to evaluate different thermodynamic models with regard to their possibility of being used for prediction of the transport properties. We performed several checks of this kind for ternary mixtures of hydrocarbons and alcohols, where extended sets of experimental data and reliable thermodynamic models were available. The sensitivity of the symmetry property to different thermodynamic parameters of the models was also checked. (C) 2003 Elsevier Science B.V. All rights reserved.
Viscosity and Density Modeling and Prediction of Reservoir Fluids: from Natural Gas to Heavy Oils

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Quiñones-Cisneros, S. E. (Ekstern), Zéberg-Mikkelsen, C. K. (Ekstern), Baylaucq, A. (Ekstern), Boned, C. (Ekstern), Stenby, E. H. (Intern)
Pages: 395-398
Publication date: 2003

Host publication information
Title of host publication: ESAT 2003
Main Research Area: Technical/natural sciences
Conference: 20th European Symposium on Applied Thermodynamics, Lahnstein, Germany, 08/10/2003 - 08/10/2003
Source: orbit
Source-ID: 209322
Publication: Research - peer-review › Article in proceedings – Annual report year: 2003

Viscosity and Liquid Density of Asymmetric Hydrocarbon Mixtures

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Queimada, A. J. (Ekstern), Cisneros, S. (Intern), Marrucho, I. M. (Ekstern), Coutinho, J. A. (Ekstern), Stenby, E. H. (Intern)
Pages: 1221-1240
Publication date: 2003
Main Research Area: Technical/natural sciences
Viscosity Modeling and Prediction of Reservoir Fluids: from Natural Gas to Heavy Oils

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Cisneros, S. (Intern), Zeberg-Mikkelsen, C. K. (Intern), Baylaucq, A. (Ekstern), Boned, C. (Ekstern), Stenby, E. H. (Intern)
Publication date: 2003

Host publication information
Title of host publication: 15th Symposium on Thermophysical Properties, Boulder, Colorado
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 41097
Publication: Research › Conference abstract in proceedings – Annual report year: 2003

VLE and VLLE Measurements of Dimethyl Ether Containing Systems. II.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Laursen, T. (Intern), Andersen, S. I. (Intern)
Pages: 1085-1087
Publication date: 2003
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal Chem Eng Data
Volume: 48
Issue number: 0
Original language: English
Source: orbit
Source-ID: 41230
Publication: Research - peer-review › Journal article – Annual report year: 2003

Whey Proteins as a Model System for Chromatographic Separation of Proteins

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Pedersen, L. (Ekstern), Mollerup, J. (Intern), Hansen, E. (Ekstern), Jungbauer, A. (Ekstern)
Pages: 161-173
Publication date: 2003
Main Research Area: Technical/natural sciences

Publication information
Journal: journal of Chromatography B
Volume: 790
Issue number: 1
ISSN (Print): 1570-0232
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 0.787 SNIP 1.033 CiteScore 2.58
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.913 SNIP 1.145 CiteScore 2.74
Web of Science (2015): Indexed yes
Accurate Density and Viscosity Modeling of Non-Polar Fluids Based on the $f$-theory

**General information**

State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Cisneros, S. (Intern), Zeberg-Mikkelsen, C. K. (Intern), Stenby, E. H. (Intern)
Pages: 41-55
Publication date: 2002
Main Research Area: Technical/natural sciences

**Publication information**

Journal: International Journal of Thermophysics
Volume: 23
Issue number: 1
ISSN (Print): 0195-928X
Ratings:
- BFI (2018): BFI-level 1
- Web of Science (2018): Indexed yes
- BFI (2017): BFI-level 1
- Web of Science (2017): Indexed Yes
- BFI (2016): BFI-level 1
- Scopus rating (2016): SJR 0.332 SNIP 0.65 CiteScore 0.83
A comment on Guggenheim-like hard-core volume expressions

**General information**

State: Published  
Organisations: Department of Chemical and Biochemical Engineering, Center for Phase Equilibria and Separation Processes, Center for Energy Resources Engineering  
Authors: Kontogeorgis, G. (Intern), Kouskoumvekaki, E. (Intern), Michelsen, M. L. (Intern)  
Pages: 4686-4688  
Publication date: 2002  
Main Research Area: Technical/natural sciences

**Publication information**

Journal: Industrial & Engineering Chemistry Research  
Volume: 41
ISSN (Print): 0888-5885
Ratings:

BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.1 SJR 0.945 SNIP 1.139
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.949 SNIP 1.146 CiteScore 2.87
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.012 SNIP 1.292 CiteScore 2.85
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 0.982 SNIP 1.243 CiteScore 2.6
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.066 SNIP 1.338 CiteScore 2.56
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.086 SNIP 1.24 CiteScore 2.58
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.047 SNIP 1.165
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.002 SNIP 1.164
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 1.142 SNIP 1.267
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.105 SNIP 1.239
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.035 SNIP 1.204
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 0.993 SNIP 1.241
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 1.046 SNIP 1.452
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 1.101 SNIP 1.266
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 1.191 SNIP 1.183
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 1.256 SNIP 1.346
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 1.372 SNIP 1.41
Web of Science (2000): Indexed yes
A Flory-Huggins model based on the Hansen Solubility Parameters

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Phase Equilibria and Separation Processes, Center for Energy Resources Engineering
Authors: Lindvig, T. (Intern), Michelsen, M. L. (Intern), Kontogeorgis, G. (Intern)
Pages: 247-260
Publication date: 2002
Main Research Area: Technical/natural sciences

Publication information
Journal: Fluid Phase Equilibria
Volume: 203
Issue number: 1
ISSN (Print): 0378-3812
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 2.33 SJR 0.869 SNIP 1.155
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.874 SNIP 0.998 CiteScore 1.99
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 0.982 SNIP 1.248 CiteScore 2.28
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.007 SNIP 1.274 CiteScore 2.31
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.152 SNIP 1.286 CiteScore 2.31
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.034 SNIP 1.234 CiteScore 2.26
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 0.986 SNIP 1.317
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.133 SNIP 1.164
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
An improved entropic expression for polymer solutions

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Kouskoumvekaki, E. (Intern), Michelsen, M. L. (Intern), Kontogeorgis, G. (Intern)
Pages: 325-335
Publication date: 2002
Main Research Area: Technical/natural sciences

Publication information
Journal: Fluid Phase Equilibria
Volume: 202
Issue number: 2
ISSN (Print): 0378-3812
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 2.33 SJR 0.869 SNIP 1.155
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.874 SNIP 0.998 CiteScore 1.99
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 0.982 SNIP 1.248 CiteScore 2.28
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.007 SNIP 1.274 CiteScore 2.31
ISI indexed (2013): ISI indexed yes
Application of the CPA Equation of State to Industrially Important Systems

General information
State: Published
Organisations: Center for Biological Sequence Analysis, Department of Systems Biology, Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Kouskoumvekaki, I. (Intern), Michelsen, M. L. (Intern), Kontogeorgis, G. (Intern)
Publication date: 2002
Event: Poster session presented at 19th European Symposium on Applied Thermodynamics, Santorini, Greece.
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 209198
Publication: Research › Poster – Annual report year: 2002

Asphaltene Self-Association: Modelling and Effect of Fractionation with a Polar Solvent

Original language: English
Source: orbit
Source-ID: 138319
Publication: Research - peer-review › Journal article – Annual report year: 2002
Detection of Occupancy Differences in Methane Gas Hydrates by Raman Spectroscopy

Diffusion in Multicomponent Mixtures

Effect of Geothermal Gradients on Fluid Distribution in Petroleum Reservoirs

Effects of Trace Water on the State of Petroleum Asphaltenes in Solution
Fractionation of Asphaltenes for Optical Analysis

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Ascanius, B. E. (Intern), Andersen, S. I. (Intern)
Publication date: 2002
Event:
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 40946
Publication: Research › Poster – Annual report year: 2002

Free-volume activity coefficient models for dendrimer solutions

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Kouskoumvekaki, E. (Intern), Giesen, R. (Ekstern), Michelsen, M. L. (Intern), Kontogeorgis, G. (Intern)
Pages: 4848-4853
Publication date: 2002
Main Research Area: Technical/natural sciences

Publication information
Journal: Industrial & Engineering Chemistry Research
Volume: 41
Issue number: 19
ISSN (Print): 0888-5885
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.1 SJR 0.945 SNIP 1.139
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.949 SNIP 1.146 CiteScore 2.87
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.012 SNIP 1.292 CiteScore 2.85
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 0.982 SNIP 1.243 CiteScore 2.6
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.066 SNIP 1.338 CiteScore 2.56
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
General one-parameter friction theory viscosity model for the Patel-Teja EOS

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Cisneros, S. (Intern), Zeberg-Mikkelsen, C. K. (Intern), Stenby, E. H. (Intern)
Publication date: 2002
Event:
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 138320
Publication: Research - peer-review › Journal article – Annual report year: 2002

High-Pressure Vapor-Liquid Equilibrium for Nitrogen + Methanol

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Phase Equilibria and Separation Processes, Center for Energy Resources Engineering
Authors: Laursen, T. (Intern), Andersen, S. I. (Intern)
Pages: 1173-1174
How to determine the pressure of a methane-containing gas mixture by means of two weak Raman bands, ν(3) and 2ν(2).

Raman spectra of a pure CH₄ sample, two CH₄-C₂H₆ mixtures and a CH₄-N₂ mixture were obtained as a function of pressure at pressures up to 39.6 MPa (MPa absolute). These spectra are presented in the region 3120-2980 cm⁻¹. A clear pressure dependence of the area ratio between two weak methane bands, n₃ (asymmetric C-H stretching) and 2n₂ (overtones of the asymmetric C-H bending), is observed; the methane n₃ band intensity is lowered relative to the methane 2n₂ as the pressure is raised. The intensity ratios between these two bands, In₃/I₂n₂, were determined and plotted as a function of pressure. Surprisingly it is observed that the ratio at a fixed pressure is independent of the composition and thereby of the surroundings in which the methane molecule is vibrating. A model function to predict the pressure is given. From a practical point of view, the present results could be useful for determining directly the total pressure in methane mixtures the composition of which is not known.

Interaction of Asphaltenes with Nonylphenol in Toluene Solutions

Interplay of Phase Behavior and Numerical Dispersion in Finite Difference Compositional Simulation
Investigation of Wax Crystallisation by FT-IR and Deuterated Trace Molecules

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Phase Equilibria and Separation Processes, Center for Energy Resources Engineering
Authors: Lindeloff, N. (Intern), Andersen, S. I. (Intern)
Publication date: 2002
Event: Poster session presented at 3rd International Conference on Petroleum Phase behavior and Fouling, New Orleans, United States.
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 40942
Publication: Research › Poster – Annual report year: 2002

Liquid-liquid equilibria for glycols plus hydrocarbons: Data and correlation
Liquid-liquid equilibrium data for seven binary glycol-hydrocarbon systems have been measured in the temperature range 32 degreesC to 80 degreesC and at the pressure 1 bar. The measured systems are monoethylene glycol (MEG) + heptane, methylecylohexane (MCH) + hexane, propylene glycol (PG) + heptane, diethylene glycol (DEG) + heptane, triethylene glycol (TEG) + heptane, and tetraethylene glycol (TETRA) + heptane. The data obtained were correlated with the NRTL model and two different versions of the UNIQUAC equation. The NRTL model and one of the UNIQUAC equations (UQ 4) have a linear temperature-dependent interaction parameter term, while the other UNIQUAC equation (UQ 2) has an interaction parameter that is independent of the temperature. There was a fairly good agreement between the experimental data and the models with an average deviation in the composition for both phases of 3% for both NRTL and UQ 4 and 15% for UQ 2. These results indicate the necessity of using the linearly dependent interaction parameters.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering, Statoil ASA
Authors: Derawi, S. (Intern), Kontogeorgis, G. (Intern), Stenby, E. H. (Intern), Haugum, T. (Ekstern), Fredheim, A. (Ekstern)
Pages: 169-173
Publication date: 2002
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Chemical and Engineering Data
Volume: 47
Issue number: 2
ISSN (Print): 0021-9568
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.29 SJR 0.88 SNIP 1.097
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.868 SNIP 0.966 CiteScore 1.96
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.021 SNIP 1.208 CiteScore 2.22
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.135 SNIP 1.199 CiteScore 2.17
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
Mass transfer properties of monoliths

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Hahn, R. (Ekstern), Panzer, M. (Ekstern), Hansen, E. (Intern), Mollerup, J. (Intern), Jungbauer, A. (Ekstern)

Publication information
Journal: Separation Science & Technology
Volume: 37
Issue number: 7
Publication date: 2002
Main Research Area: Technical/natural sciences

Original language: English
DOIs: 10.1021/je010199a
Source: orbit
Source-ID: 138321
Publication: Research - peer-review › Journal article – Annual report year: 2002
Modeling of heavy metal salt solubility using the Extended UNIQUAC model

Solid-liquid equilibria in complex aqueous systems involving a heavy metal cation (Mn²⁺, Fe²⁺, Co²⁺, Ni²⁺, Cu²⁺, or Zn²⁺) and one or more ions for which Extended UNIQUAC parameters have been published previously are modeled using the Extended UNIQUAC model. Model parameters are determined on the basis of a data bank with more than 4,000 experimental data points for binary and ternary aqueous systems. The parameters are generally valid in the temperature range from the freezing point to the boiling point of the respective solutions.

General information
State: Published
Modelling the Acid Restimulation of Carbonate Fractured Injection Wells in a North Sea

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Phase Equilibria and Separation Processes, Center for Energy Resources Engineering
Authors: Berenblyum, R. (Intern), Hansen, J. H. (Ekstern), Michelsen, M. L. (Intern), Shapiro, A. (Intern), Stenby, E. H. (Intern)
Publication date: 2002
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 209318
Publication: Research › Conference abstract for conference – Annual report year: 2002

Phase Equilibria for Complex Polymer Solutions
Many commercially important mixtures contain complex polymers, e.g. paints and coatings. If a good thermodynamic description can be given of these systems it is possible to develop paints, which possess a certain set of properties and at the same time meet some basic requirement as, e.g. regarding the content of organic solvents.

This work presents an investigation of the three polymer models Entropic-FV (EFV), UNIFAC-FV (UFV) and GC-Flory (GCF) for their capability of predicting solvent activity coefficients in binary systems containing complex polymers. It is possible to obtain good predictions at finite concentrations and satisfactory predictions at infinite dilution, particularly with the EFV model. The investigation shows that EFV is the most robust and stable of the models, which indicates that it is the most well suited model for further development of methods for predicting the miscibility behavior of paints and related systems. (C) 2002 Elsevier Science B.V. All rights reserved.
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 2.33 SJR 0.869 SNIP 1.155
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.874 SNIP 0.998 CiteScore 1.99
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 0.982 SNIP 1.248 CiteScore 2.28
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.007 SNIP 1.274 CiteScore 2.31
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.152 SNIP 1.286 CiteScore 2.31
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.034 SNIP 1.234 CiteScore 2.26
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 0.986 SNIP 1.317
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.133 SNIP 1.164
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.227 SNIP 1.09
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.031 SNIP 1.151
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.034 SNIP 1.245
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.009 SNIP 1.3
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 0.985 SNIP 1.349
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 1.193 SNIP 1.301
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 0.722 SNIP 1.101
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 0.966 SNIP 1.284
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 0.87 SNIP 0.898
Web of Science (2000): Indexed yes
Scopus rating (1999): SJR 0.938 SNIP 0.885

Original language: English
Thermodynamics, Polymers, Paints, Activity coefficients, Group contribution, Mixture
DOI: 10.1016/S0378-3812(01)00715-4
Prediction of Gas Solubilities in Elastomeric Polymers for the Design of Thermopane Windows

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, Center for Phase Equilibria and Separation Processes, Center for Energy Resources Engineering
Authors: Thorlaksen, P. (Ekstern), Abildskov, J. (Ekstern), Kontogeorgis, G. (Intern)
Pages: 17-33
Publication date: 2002
Main Research Area: Technical/natural sciences

Publication information
Journal: Fluid Phase Equilibria
Volume: 211
Issue number: 2003
ISSN (Print): 0378-3812
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 2.33 SJR 0.869 SNIP 1.155
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.874 SNIP 0.998 CiteScore 1.99
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 0.982 SNIP 1.248 CiteScore 2.28
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.007 SNIP 1.274 CiteScore 2.31
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.152 SNIP 1.286 CiteScore 2.31
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.034 SNIP 1.234 CiteScore 2.26
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 0.986 SNIP 1.317
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.133 SNIP 1.164
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.227 SNIP 1.09
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.031 SNIP 1.151
Prediction of micelle formation for aqueous polyoxyethylene alcohol solutions with the UNIFAC model

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Cheng, H. (Intern), Kontogeorgis, G. (Intern), Stenby, E. H. (Intern)
Pages: 892-898
Publication date: 2002
Main Research Area: Technical/natural sciences

Publication information
Journal: Industrial & Engineering Chemistry Research
Volume: 41
Issue number: 5
ISSN (Print): 0888-5885
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.1 SJR 0.945 SNIP 1.139
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.949 SNIP 1.146 CiteScore 2.87
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.012 SNIP 1.292 CiteScore 2.85
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 0.982 SNIP 1.243 CiteScore 2.6
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.066 SNIP 1.338 CiteScore 2.56
Prediction of Octanol-Water Partition Coefficients of Surfactants with Engineering Methods

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Cheng, H. (Intern), Kontogeorgis, G. (Intern), Stenby, E. H. (Intern)
Publication date: 2002

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 40871
Publication: Research - peer-review › Journal article – Annual report year: 2002

Principle of Entropy Maximization for Nonequilibrium Steady States
The goal of this contribution is to find out to what extent the principle of entropy maximization, which serves as a basis for the equilibrium thermodynamics, may be generalized onto non-equilibrium steady states. We prove a theorem that, in the system of thermodynamic coordinates, where entropy has a maximum in a steady state with regard to some thermodynamic variables, the matrix of the Onsager phenomenological coefficients becomes diagonal. The theorem requires consistent rules of the coordinate transformations in the non-equilibrium thermodynamics. Such rules are
formulated. The results make it possible, in some cases, to reduce the number of unknown transport coefficients in thermodynamic description of the transport processes.

**General information**
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Shapiro, A. (Intern), Stenby, E. H. (Intern)
Pages: 61-73
Publication date: 2002
Main Research Area: Technical/natural sciences

**Publication information**
Journal: Lecture Notes in Physics
Volume: 584
ISSN (Print): 1616-6361
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 0.591 SNIP 0.382 CiteScore 0.55
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.661 SNIP 0.428 CiteScore 0.8
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.815 SNIP 0.509 CiteScore 1.12
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.542 SNIP 0.426 CiteScore 0.75
ISI indexed (2013): ISI indexed no
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.363 SNIP 0.36 CiteScore 0.48
ISI indexed (2012): ISI indexed no
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.396 SNIP 0.288 CiteScore 0.53
ISI indexed (2011): ISI indexed no
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.44 SNIP 0.339
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.414 SNIP 0.314
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.278 SNIP 0.212
Scopus rating (2007): SJR 0.22 SNIP 0.172
Scopus rating (2006): SJR 0.297 SNIP 0.25
Scopus rating (2004): SJR 0.122 SNIP 0
Scopus rating (2003): SJR 0.121 SNIP 0
Scopus rating (2002): SJR 0.121 SNIP 0
Original language: English
DOIs:
10.1007/3-540-45791-7_4
Source: orbit
Source-ID: 250800
Publication: Research - peer-review › Journal article – Annual report year: 2002

**Produktion af gødningssalte**

**General information**
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Phase Equilibria and Separation Processes, Center for Energy Resources Engineering
Authors: Christensen, S. G. (Intern), Thomsen, K. (Intern)
Scale Formation in Geothermal Plants

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Garcia, A. V. (Ekstern), Thomsen, K. (Intern), Stenby, E. H. (Intern)
Publication date: 2002

Screening Vapor Pressure Data

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Olsen, E. (Ekstern), Kontogeorgis, G. (Intern)
Publication date: 2002

Sequential algorithm for calculating ordinary critical points

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Cisneros, S. (Intern), Valle-Arizmedi, L. (Ekstern), Barragán-Aroche, F. (Ekstern), Bazúa-Rueda, E. (Ekstern)
Publication date: 2002
Sodium Chloride Dihydrate - A Potential Cause of Slippery Accidents

From a thermodynamic point of view, it can be expected that sodium chloride dihydrate (hydrohalite, NaCl2H2O) will form on winter roads under certain conditions at temperatures below 0.1°C. In order to elucidate whether or not the formation of hydrohalite on the pavement can explain the phenomenon of ice appearing to be resistant to road salt, a comparative study has been made on a number of different surfaces measuring the friction index. The friction measurements were performed with a Portable Skid-Resistance Tester. Discontinuous surfaces consisting of small islands of hydrohalite was classified as potentially slippery surfaces. It is therefore possible that the formation of hydrohalite contributes to accidents on slippery roads.

Study On The Self-Association Of Asphaltenes And Their Interaction With Resins By Calorimetry

Surface tension of heptane, decane, hexadecane, eicosane, and some of their binary mixtures

Surface tension measurements were performed by the Wilhelmy plate method. Measured systems included pure heptane, decane, hexadecane, eicosane, and some of their binary mixtures at temperatures from 293.15 K to 343.15 K with an average absolute deviation of 1.6%. The results were compared with a new corresponding states model. The average absolute deviation was found to be 1.0%.
Thermodynamics of polymer solutions (16th chapter)

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Kontogeorgis, G. (Intern)
Publication date: 2002

Host publication information
Title of host publication: Handbook of Colloid and Surface Chemistry, 2nd edition
Publisher: CRC Press
Edition: 2
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 138314
Publication: Research - peer-review › Book chapter – Annual report year: 2003

Trace Water-Asphaltene Interaction in Organic Solvents

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Khvostichenko, D. S. (Ekstern), Victorov, A. (Ekstern), Andersen, S. I. (Intern)
Publication date: 2002
Event: Poster session presented at 2002 Heavy Organic Deposition International Conference, Puerto Vallarta, Mexico.
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 40944
Publication: Research › Poster – Annual report year: 2002

Viscosity modeling and prediction of crude oils

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Cisneros, S. (Intern), Stenby, E. H. (Intern)
Publication date: 2002
Event:
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 40954
Publication: Research › Conference abstract for conference – Annual report year: 2002

Viscosity modeling of associating fluids based on the friction theory: pure alcohols

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Zeberg-Mikkelsen, C. K. (Intern), Cisneros, S. (Intern), Stenby, E. H. (Intern)
Pages: 1191-1203
Publication date: 2002
Main Research Area: Technical/natural sciences

Publication information
Journal: Fluid Phase Equilibria
Volume: 194
Issue number: 0
ISSN (Print): 0378-3812
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 2.33 SJR 0.869 SNIP 1.155
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.874 SNIP 0.998 CiteScore 1.99
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 0.982 SNIP 1.248 CiteScore 2.28
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.007 SNIP 1.274 CiteScore 2.31
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.152 SNIP 1.286 CiteScore 2.31
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.034 SNIP 1.234 CiteScore 2.26
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 0.986 SNIP 1.317
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.133 SNIP 1.164
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.227 SNIP 1.09
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.031 SNIP 1.151
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.034 SNIP 1.245
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.009 SNIP 1.3
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 0.985 SNIP 1.349
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 1.193 SNIP 1.301
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 0.722 SNIP 1.101
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 0.966 SNIP 1.284
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 0.87 SNIP 0.898
Web of Science (2000): Indexed yes
Scopus rating (1999): SJR 0.938 SNIP 0.885

Original language: English
Source: orbit
Source-ID: 40864
Viscosity Modelling of Four Polar Fluids Based on the Friction Theory and the Free-Volume Theory

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Comuñas, M. J. P. (Ekstern), Baylaucq, A. (Ekstern), Quiñones-Cisneros, S. E. (Ekstern), Zeberg-Mikkelsen, C. K. (Intern), Boned, C. (Ekstern), Fernández, J. (Ekstern)
Publication date: 2002
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 209317
Publication: Research › Conference abstract for conference – Annual report year: 2002

Viscosity prediction of carbon dioxide plus hydrocarbon mixtures using the friction theory
The general one-parameter f-theory model has been used in conjunction with the SRK and the PR EOS to predict the viscosity of well-defined carbon dioxide + hydrocarbon mixtures. The predicted viscosities are within the uncertainty appropriate for most industrial applications. Although the studied mixtures are simple representations or real oil mixtures with carbon dioxide, the f-theory approach can easily be extended to more complex scenarios, such as the simulation of carbon dioxide enhance oil recovery. Additionally, a comparison with the LBC model, which is a widely used model in the oil industry, has been carried Out. In contrast to the f-theory models, the strong dependency that the LBC model has on the accuracy or the density is clearly evident for the kind of Mixtures Studied in this work. Furthermore, it is shown how the phase behavior complexity that carbon dioxide + hydrocarbon mixtures develop may have a direct influence on the performance of the viscosity modeling and prediction.

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Zeberg-Mikkelsen, C. K. (Intern), Cisneros, S. (Intern), Stenby, E. H. (Intern)
Pages: 27-42
Publication date: 2002
Main Research Area: Technical/natural sciences

Publication information
Journal: Petroleum Science and Technology
Volume: 20
Issue number: 1
ISSN (Print): 1091-6466
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 0.285 SNIP 0.508 CiteScore 0.6
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.265 SNIP 0.584 CiteScore 0.48
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.296 SNIP 0.774 CiteScore 0.4
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.411 SNIP 0.851 CiteScore 0.48
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.271 SNIP 0.565 CiteScore 0.38
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Viscosity Prediction of Natural Gas Using the Friction Theory

Based on the concepts of the friction theory (f-theory) for viscosity modeling, a procedure is introduced for predicting the viscosity of hydrocarbon mixtures rich in one component, which is the case for natural gases. In this procedure, the mixture friction coefficients are estimated with mixing rules based on the values of the pure component friction coefficients. Since natural gases contain mainly methane, two f-theory models are combined, where the friction coefficients of methane are estimated by a seven-constant f-theory model directly fitted to methane viscosities, and the friction coefficients of the other components are estimated by the one-parameter general f-theory model. The viscosity predictions are performed with the SRK, the PR, and the PRSV equations of state, respectively. For recently measured viscosities of natural gases, the resultant AAD (0.5 to 0.8%) is in excellent agreement with the experimental uncertainty (+/-1.0%). The AAD is found to be higher for older measurements (around 3.5%), due mainly to the higher experimental uncertainties and problems with some of the measurements. Overall, the results are satisfactory for most industrial applications related to natural gases.
VLE and VLLE measurements of dimethyl ether containing systems

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Phase Equilibria and Separation Processes, Center for Energy Resources Engineering
Application of Group Contribution Models to the Calculation of the Octanol-Water Partition Coefficient

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Derawi, S. (Ekstern), Kontogeorgis, G. (Intern), Stenby, E. H. (Ekstern)
Pages: 434-443
Publication date: 2001
Main Research Area: Technical/natural sciences

Publication information
Journal: Industrial & Engineering Chemistry Research
Volume: 40
Issue number: 1
ISSN (Print): 0888-5885
Ratings:
A Thermodynamic Model for Gas Hydrates in the Presence of Salts and Methanol

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Zuo, Y. (Ekstern), Zhang, D. (Ekstern), Stenby, E. H. (Intern)
Pages: 175-192
Publication date: 2001
Main Research Area: Technical/natural sciences

Publication information
Journal: Chemical Engineering Communications
Volume: 184
ISSN (Print): 0098-6445
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.28 SJR 0.338 SNIP 0.803
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.383 SNIP 0.829 CiteScore 1.28
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.404 SNIP 0.791 CiteScore 1.2
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.411 SNIP 0.729 CiteScore 1.05
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.404 SNIP 0.813 CiteScore 1.15
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.421 SNIP 0.646 CiteScore 1.01
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.423 SNIP 0.566
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.337 SNIP 0.519
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.369 SNIP 0.535
Scopus rating (2007): SJR 0.313 SNIP 0.365
Scopus rating (2006): SJR 0.249 SNIP 0.553
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 0.345 SNIP 0.498
Scopus rating (2004): SJR 0.32 SNIP 0.5
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 0.346 SNIP 0.341
Scopus rating (2002): SJR 0.413 SNIP 0.514
Scopus rating (2001): SJR 0.429 SNIP 0.472
A Wax Inhibition Solution to Problematic Fields: A Chemical Remediation Process

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Groffe, D. (Ekstern), Groffe, P. (Ekstern), Takhar, S. (Ekstern), Andersen, S. I. (Intern), Stenby, E. H. (Intern), Lindeloff, N. (Ekstern)
Pages: 205-217
Publication date: 2001
Main Research Area: Technical/natural sciences

Publication information
Journal: Petroleum Science and Technology
Volume: 19
Issue number: 1
ISSN (Print): 1091-6466
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 0.285 SNIP 0.508 CiteScore 0.6
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.265 SNIP 0.584 CiteScore 0.48
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.296 SNIP 0.774 CiteScore 0.4
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.411 SNIP 0.851 CiteScore 0.48
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.271 SNIP 0.565 CiteScore 0.38
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.322 SNIP 0.637 CiteScore 0.5
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.27 SNIP 0.439
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.362 SNIP 0.544
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.283 SNIP 0.497
Scopus rating (2007): SJR 0.265 SNIP 0.484
Scopus rating (2006): SJR 0.327 SNIP 0.46
Scopus rating (2005): SJR 0.345 SNIP 0.572
Web of Science (2005): Indexed yes
Characterization of Asphaltenes and Resins from Problematic Mexican Crude Oils

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Buenrostro-Gonzalez, E. (Ekstern), Espinosa-Peñ, M. (Ekstern), Andersen, S. I. (Intern)
Pages: 299-316
Publication date: 2001
Main Research Area: Technical/natural sciences

Publication information
Journal: Petroleum Science and Technology
Volume: 19
Issue number: 3-4
ISSN (Print): 1091-6466
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 0.285 SNIP 0.508 CiteScore 0.6
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.265 SNIP 0.584 CiteScore 0.48
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.296 SNIP 0.774 CiteScore 0.4
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.411 SNIP 0.851 CiteScore 0.48
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.271 SNIP 0.565 CiteScore 0.38
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.322 SNIP 0.637 CiteScore 0.5
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.27 SNIP 0.439
Chemical Product Engineering - A Cross-centre Activity at Institut for Kemiteknik

General information
State: Published
Organisations: CHEC Research Centre, Department of Chemical and Biochemical Engineering, Center for Phase Equilibria and Separation Processes, Computer Aided Process Engineering Center, The Danish Polymer Centre, The Aerosol Laboratory, Center for Energy Resources Engineering
Publication date: 2001
Event: Poster session presented at Conference on Refocusing Chemical Engineering, Barga, Italy.
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 40989
Publication: Research - peer-review › Journal article – Annual report year: 2001

Density and viscosity of the 1-methylnaphthalene+2,2,4,4,6,8,8-heptamethylnonane system from 293.15 to 353.15 K at pressures up to 100 Mpa

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Phase Equilibria and Separation Processes, Center for Energy Resources Engineering
Authors: Canet, X. (Ekstern), Dauge, P. (Ekstern), Baylaucq, A. (Ekstern), Boned, C. (Ekstern), Zeberg-Mikkelsen, C. K. (Intern), Quiñones-Cisneros, S. E. (Ekstern), Stenby, E. H. (Intern)
Pages: 1669-1689
Publication date: 2001
Main Research Area: Technical/natural sciences

Publication information
Journal: International Journal of Thermophysics
Volume: 22
Issue number: 6
ISSN (Print): 0195-928X
Determination of the activity coefficients of glycylglycine and glycyl-L-alanine in sodium chloride solutions by an electrochemical cell with ion-selective electrodes: Experimental measurements and

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Development of Petroleum Enhanced Coal Tar Pitch in Europe

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Pages: 565-572
Publication date: 2001

Host publication information
Title of host publication: TMS Annual Meeting, New Orleans, Louisiana, February, 2001
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 40998
Publication: Research › Conference abstract in proceedings – Annual report year: 2001

Estimation of VLE Phase Compositions of Binary Systems Containing Gaseous Components, from the Feed Composition and the Cell Volume

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Soave, G. (Ekstern), Colussi, S. (Ekstern), Stenby, E. H. (Intern)
Pages: 373-389
Publication date: 2001
Main Research Area: Technical/natural sciences

Publication information
Journal: Fluid Phase Equilibria
Volume: 187-188
ISSN (Print): 0378-3812
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 2.33 SJR 0.869 SNIP 1.155
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.874 SNIP 0.998 CiteScore 1.99
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 0.982 SNIP 1.248 CiteScore 2.28
High-Pressure Vapor-Liquid Equilibria in the Systems: nitrogen + dimethyl ether, methanol + dimethyl ether, carbon dioxide + dimethyl ether + methanol and nitrogen + dimethyl ether + methanol

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Teodorescu, M. (Ekstern), Rasmussen, P. (Intern)
Pages: 640-646
Publication date: 2001
Main Research Area: Technical/natural sciences
High Pressure Viscosity and Density Behaviour of Ternary Mixtures: 1-Methylnaphthalene + n-Tridecane + 2,2,4,4,6,8,8-Heptamethylnonane

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Zeberg-Mikkelsen, C. K. (Intern), Canet, X. (Ekstern), Baylaucq, A. (Ekstern), Cisneros, S. (Intern), Boned, C. (Ekstern), Stenby, E. H. (Intern)
Pages: 1691-1726
Publication date: 2001
Main Research Area: Technical/natural sciences

Publication information
Journal: International Journal of Thermophysics
Volume: 22
Issue number: 6
ISSN (Print): 0195-928X
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 0.332 SNIP 0.65 CiteScore 0.83
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.39 SNIP 0.979 CiteScore 0.9
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.466 SNIP 1.104 CiteScore 1.02
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.401 SNIP 1.311 CiteScore 1.13
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.371 SNIP 0.752 CiteScore 0.77
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.532 SNIP 1.112 CiteScore 1.08
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.455 SNIP 0.798
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.459 SNIP 0.849
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.563 SNIP 0.92
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 0.599 SNIP 0.915
Interaction and Solubilization of Water by Petroleum Asphaltenes in Organic Solution

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Andersen, S. I. (Intern), Manuel del Rio-Garcia, J. (Ekstern), Khovstitchenko, D. (Ekstern), Shakir*, S. (Ekstern), Lira-Galeana, C. (Ekstern)
Pages: 307-313
Publication date: 2001
Main Research Area: Technical/natural sciences

Publication information
Journal: Langmuir
Volume: 17
Issue number: 2
ISSN (Print): 0743-7463
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.99 SJR 1.55 SNIP 1.188
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.686 SNIP 1.308 CiteScore 4.33
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.816 SNIP 1.391 CiteScore 4.59
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.895 SNIP 1.356 CiteScore 4.55
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 2.177 SNIP 1.382 CiteScore 4.37
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
Investigations of Inhibition of Asphaltene Precipitation at High Pressure Using Bottomhole Samples

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Aquino-Olivos, M. (Ekstern), Buenrostro-Gonzalez, E. (Ekstern), Andersen, S. I. (Intern), Lira-Galeana, C. (Ekstern)
Pages: 236-240
Publication date: 2001
Main Research Area: Technical/natural sciences

Publication information
Journal: Energy & Fuels
Volume: 15
Issue number: 1
ISSN (Print): 0887-0624
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
Measurement and modeling of the solubility of CO2 and N2 in a model resin system based on resin from spruce wood (Picea abies (L))

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Phase Equilibria and Separation Processes, Center for Energy Resources Engineering
Authors: Laursen, T. (Intern), Andersen, S. I. (Intern), Dahl, S. (Ekstern), Henriksen, O. (Ekstern)
Pages: 239-250
Publication date: 2001
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Supercritical Fluids
Volume: 19
Original language: English
Source: orbit

Original language: English
Source: orbit
Source-ID: 40986
Publication: Research - peer-review › Journal article – Annual report year: 2001
Novel Applications of Thermodynamics with Classical Models

General information
State: Published
Organisations: Department of Applied Chemistry, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Lindvig, T. (Intern), Derawi, S. (Intern), Hansen, C. (Intern), Michelsen, M. L. (Intern), Stenby, E. H. (Intern), Kontogeorgis, G. (Intern)
Publication date: 2001

Host publication information
Title of host publication: 3. Greek Scientific Conference of Chemical Engineering, Athens, Greece, 01/01/2001
Main Research Area: Technical/natural sciences
Fluid Phase Equilibria 194-197 (2002) p 663-673
Source: orbit
Source-ID: 41002
Publication: Research › Conference abstract in proceedings – Annual report year: 2001

One Parameter Friction Theory Models for Viscosity

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Cisneros, S. (Intern), Zeberg-Mikkelsen, C. K. (Intern), Stenby, E. H. (Intern)
Pages: 1-16
Publication date: 2001
Main Research Area: Technical/natural sciences

Publication information
Journal: Fluid Phase Equilibria
Volume: 178
Issue number: 1
ISSN (Print): 0378-3812
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 2.33 SJR 0.869 SNIP 1.155
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.874 SNIP 0.998 CiteScore 1.99
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 0.982 SNIP 1.248 CiteScore 2.28
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.007 SNIP 1.274 CiteScore 2.31
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.152 SNIP 1.286 CiteScore 2.31
ISI indexed (2012): ISI indexed yes
On the Mass Balance of Asphaltene Precipitation

In the evaluation of experimental data as well as in calculation of phase equilibria the necessity of the application of mass balances is obvious. In the case of asphaltenes the colloidal nature of these compounds may highly affect the mass balance. In the present paper several experiments are performed in order to check the consistency of mass balances within asphaltene precipitation. Asphaltenes are precipitated in two step processes either by changing temperature or by changes in precipitant with increasing precipitation power. This has been performed for three different oils. The data indicates that in temperature experiments as well as in solvent series experiments the precipitation of heavy asphaltenes affects the following precipitation of lighter asphaltenes. In both cases the mass balance using standard separation techniques cannot be closed, as less material is precipitated in a two step process than in the direct process either at low temperature or by direct precipitation with one precipitant. The different fractions were subject to HPLC size exclusion chromatography showing that the material remaining in solution in the stepwise process was of low molecular weight, and that the material in the second precipitation step was often of higher apparent molecular weight anti had an increased overall absorbance coefficient.

General information

State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Andersen, S. I. (Intern), Lira-Galeana, C. (Ekstern), Stenby, E. H. (Intern)
Pages: 457-467
Publication date: 2001
Main Research Area: Technical/natural sciences
Organic Precipitates in Oil Production of a Venezuelan Oil Field

**General information**

State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Andersen, S. I. (Intern), Hofsäss, T. (Ekstern), Kleinitz, W. (Ekstern), Rahimian, I. (Ekstern)
Pages: 55-74
Publication date: 2001
Main Research Area: Technical/natural sciences

**Publication information**

Journal: Petroleum Science and Technology
Volume: 19
Issue number: 1 & 2
ISSN (Print): 1091-6466
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 0.285 SNIP 0.508 CiteScore 0.6
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.265 SNIP 0.584 CiteScore 0.48
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.296 SNIP 0.774 CiteScore 0.4
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.411 SNIP 0.851 CiteScore 0.48
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.271 SNIP 0.565 CiteScore 0.38
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.322 SNIP 0.637 CiteScore 0.5
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.27 SNIP 0.439
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.362 SNIP 0.544
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.283 SNIP 0.497
Scopus rating (2007): SJR 0.265 SNIP 0.484
Scopus rating (2006): SJR 0.327 SNIP 0.46
Scopus rating (2005): SJR 0.345 SNIP 0.572
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 0.396 SNIP 0.689
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 0.311 SNIP 0.458
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 0.467 SNIP 0.581
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 0.619 SNIP 0.941
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 0.535 SNIP 0.764
Web of Science (2000): Indexed yes
Petroleum Resins: Separation, Character, and Role in Petroleum

In petroleum science, the term resin generally implies material that has been eluted from various solid adsorbents, whereas the term maltenes (or petrolenes) indicates a mixture of the resins and oils obtained as filtrates from the asphaltene precipitation. Thus, after the asphaltenes are precipitated, adsorbents are added to the n-pentane solutions of the resins and oils, by which process the resins are adsorbed and subsequently recovered by the use of a more polar solvent, and the oils remain in solution. The resin fraction plays an important role in the stability of petroleum and prevents separation of the asphaltene constituents as a separate phase. Indeed, the absence of the resin fraction (produced by a variety of methods) from the maltenes influences the ability of the de-resined maltenes to accommodate the asphaltenes either in solution or as a stable part of a colloidal system. In spite of the fact that the resin fraction is extremely important to the stability of petroleum, there is surprisingly little work reported on the characteristics of the resins. This article summarizes the work that has been carried out in determining the character and properties of the resin constituents. Suggestions are also made regarding current thoughts of the role of these constituents on the structure and stability of petroleum.
Physical Properties from Association Models

**General information**
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering, Shell Global Solutions
Authors: Michelsen, M. L. (Intern), Hendriks, E. M. (Ekstern)
Pages: 165-174
Publication date: 2001
Main Research Area: Technical/natural sciences

**Publication information**
Journal: Fluid Phase Equilibria
Volume: 180
ISSN (Print): 0378-3812
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 2.33 SJR 0.869 SNIP 1.155
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.874 SNIP 0.998 CiteScore 1.99
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 0.982 SNIP 1.248 CiteScore 2.28
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.007 SNIP 1.274 CiteScore 2.31
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.152 SNIP 1.286 CiteScore 2.31
Prediction of the Surface Tension of Hydrocarbons and Their Mixtures

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Phase Equilibria and Separation Processes, Center for Energy Resources Engineering
Authors: Queimada, A. (Intern), Coutinho, J. (Intern), Marrucho, I. M. (Ekstern), Kontogeorgis, G. (Intern), Stenby, E. H. (Intern)
Publication date: 2001

Host publication information
Title of host publication: Chempor 2001
Main Research Area: Technical/natural sciences
Conference: Chempor 2001 - 8th International Conference in chemical Engineering, Aveiro, Portugal, 01/01/2001
Source: orbit
Source-ID: 40981
Publication: Research - peer-review › Journal article – Annual report year: 2001

Raman Spectroscopic Studies of Methane-Ethane Mixtures as a Function of Pressure
Raman spectra of methane and methane-ethane mixtures (100, 85, and 49 mole % CH4) have been obtained as a function of pressure in the pressure range 0.1 to 15.3 MPaA (MPa absolute). For these mixtures methane nu (1)
(symmetric C-H stretching) band positions are given as a function of pressure; for pure methane they are in agreement with previous results. The new data on the methane ν (1) band position of ethane-containing mixtures clearly depend on the kind of molecules surrounding the vibrating methane molecule. The ν (1) band position decreases with increasing pressure; the stronger the dependency, the higher the content of ethane. The ethane ν (1) band position in the two mixtures showed the same kind of dependency. A qualitative explanation for this behavior is attempted, relating it to changes in van der Waals-type interactions on pressure.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Department of Chemistry, Center for Phase Equilibria and Separation Processes, Center for Energy Resources Engineering
Authors: Hansen, S. B. (Intern), Berg, R. W. (Intern), Stenby, E. H. (Intern)
Pages: 745-749
Publication date: 2001
Main Research Area: Technical/natural sciences

Publication information
Journal: Applied Spectroscopy
Volume: 55
Issue number: 6
ISSN (Print): 0003-7028
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
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BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.649 SNIP 1.09 CiteScore 1.96
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.619 SNIP 1.077 CiteScore 1.96
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.627 SNIP 1.162 CiteScore 2.08
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.581 SNIP 1.103 CiteScore 1.81
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.6 SNIP 1.031 CiteScore 1.62
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.687 SNIP 0.989
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.634 SNIP 0.907
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.85 SNIP 1.09
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 0.772 SNIP 0.992
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 0.795 SNIP 1.004
Size Exclusion Chromatography in the Analysis of Pitch

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Ascanius, B. E. (Intern), Malmros, O. (Ekstern), Turner, N. R. (Ekstern), Stenby, E. H. (Intern), Andersen, S. I. (Intern)
Pages: 559-564
Publication date: 2001

Host publication information
Title of host publication: TMS Annual Meeting, New Orleans, Louisiana, February, 2001
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 40997
Publication: Research - peer-review › Conference abstract in proceedings – Annual report year: 2001

Studies of waterflooding in low-permeable chalk by use of X-ray CT scanning

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Phase Equilibria and Separation Processes, Center for Energy Resources Engineering
Authors: Mogensen, K. (Intern), Stenby, E. H. (Intern), Zhou, D. Z. (Ekstern)
Pages: 1-10
Publication date: 2001
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Petroleum Science and Engineering
Volume: 32
ISSN (Print): 0920-4105
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.56 SJR 0.764 SNIP 1.631
The Friction Theory for Viscosity Modeling: Extension to Crude Oil Systems

In this work the one-parameter friction theory (f-theory) general models have been extended to the viscosity prediction and modeling of characterized oils. It is demonstrated that these simple models, which take advantage of the repulsive and attractive pressure terms of cubic equations of state such as the SRK, PR and PRSV, can provide accurate viscosity prediction and modeling of characterized oils. In the case of light reservoir oils, whose properties are close to those of normal alkanes, the one-parameter f-theory general models can predict the viscosity of these fluids with good accuracy. Yet, in the case when experimental information is available a more accurate modeling can be obtained by means of a simple tuning procedure. A tuned f-theory general model can deliver highly accurate viscosity modeling above the saturation pressure and good prediction of the liquid-phase viscosity at pressures below the saturation pressure. In addition, a tuned f-theory general model delivers accurate modeling of different kinds of light and heavy oils. Thus, the simplicity and stability of the f-theory general models make them a powerful tool for applications such as reservoir simulations, between others. (C) 2001 Elsevier Science Ltd. All rights reserved.
Thermodynamics of Paint Related Systems with Engineering Models

Paints are complex materials composed of polymers (binders) dissolved in one or more solvents, pigments, and other additives. The thermodynamics of such systems is essential, for example, for selecting improved solvents and understanding a number of phenomena related especially to adhesion to solid surfaces and drying. Many engineering models have been applied over the last decades for solutions with commodity polymers. In this work the performance of some of these models is investigated for paint-related systems, focusing on those drying by the so-called "lacquer mechanism" (evaporation of solvents). These are the Entropic-FV UNIFAC-FV, GC-Flory, and the Flory-Huggins models using various ways for estimating the FH parameter via solubility, parameters. Achievements and shortcomings of these models are discussed in conjunction with difficulties encountered in such calculations. We conclude that, despite the uncertainties involved, several models yield reasonably accurate activity coefficients, even at infinite dilution. Thus, engineering models may be useful for solvent selection via semiempirical rules of thumb, which are based on thermodynamic considerations.

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Lindvig, T. (Intern), Michelsen, M. L. (Intern), Kontogeorgis, G. (Intern)
Pages: 2573-2584
Publication date: 2001
Main Research Area: Technical/natural sciences

Publication information
Journal: A I Ch E Journal
Volume: 47
Issue number: 11
ISSN (Print): 0001-1541
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.11 SJR 1.034 SNIP 1.268
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.085 SNIP 1.417 CiteScore 3.03
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.07 SNIP 1.332 CiteScore 2.86
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.05 SNIP 1.364 CiteScore 2.59
### Viscosity Modeling of Light Gases at Supercritical Conditions Using the Friction Theory

**General information**

State: Published  
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering  
Authors: Zeberg-Mikkelsen, C. K. (Intern), Cisneros, S. (Intern), Stenby, E. H. (Intern)  
Pages: 3848-3854  
Publication date: 2001  
Main Research Area: Technical/natural sciences

**Publication information**

Journal: I&EC Research  
Volume: 40  
Issue number: 17

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Viscosity modeling of the ternary system 1-methylnaphthalene plus n-tridecane+ 2,2,4,4,6,8,8-heptamethylnonane up to 100 Mpa

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Zeberg-Mikkelsen, C. K. (Intern), Canet, X. (Ekstern), Cisneros, S. (Intern), Baylaucq, A. (Ekstern), Allal, A. (Ekstern), Boned, C. (Ekstern), Stenby, E. H. (Intern)
Pages: 281-303
Publication date: 2001
Main Research Area: Technical/natural sciences

Publication information
Journal: High Pressure Research
Volume: 21
ISSN (Print): 0895-7959
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.12 SJR 0.437 SNIP 0.724
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.459 SNIP 0.889 CiteScore 1.08
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.499 SNIP 0.688 CiteScore 0.99
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.448 SNIP 0.648 CiteScore 1.03
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.461 SNIP 0.5 CiteScore 0.82
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.688 SNIP 0.71 CiteScore 0.95
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.736 SNIP 0.765
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.575 SNIP 0.643
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.587 SNIP 0.762
Scopus rating (2007): SJR 0.788 SNIP 0.746
Scopus rating (2006): SJR 0.585 SNIP 0.599
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 0.45 SNIP 0.374
Scopus rating (2004): SJR 0.328 SNIP 0.322
Viscosity Prediction of Hydrocarbon Mixtures Based on the Friction Theory

The application and capability of the friction theory (f-theory) for viscosity predictions of hydrocarbon fluids is further illustrated by predicting the viscosity of binary and ternary liquid mixtures composed of n-alkanes ranging from n-pentane to n-decane for wide ranges of temperature and from low to high pressures. In the f-theory viscosity predictions the SRK and the PRSV EOS have respectively been used. Further, a comparison with the widely used LBC viscosity model shows that better results are obtained with the f-theory models. The obtained AAD% is within or close to the experimental uncertainty, which is satisfactorily for most applications related to the oil industry.

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Zeberg-Mikkelsen, C. K. (Intern), Cisneros, S. (Intern), Stenby, E. H. (Intern)
Pages: 899-910
Publication date: 2001
Main Research Area: Technical/natural sciences

Publication information
Journal: Petroleum Science and Technology
Volume: 19
Issue number: 7
ISSN (Print): 1091-6466
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 0.285 SNIP 0.508 CiteScore 0.6
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.265 SNIP 0.584 CiteScore 0.48
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.296 SNIP 0.774 CiteScore 0.4
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.411 SNIP 0.851 CiteScore 0.48
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.271 SNIP 0.565 CiteScore 0.38
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.322 SNIP 0.637 CiteScore 0.5
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.27 SNIP 0.439
BFI (2009): BFI-level 1
Viscosity Prediction of Hydrogen + Natural Gas Mixtures (Hythane)

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Zeberg-Mikkelsen, C. K. (Intern), Cisneros, S. (Intern), Stenby, E. H. (Intern)
Pages: 2966-2970
Publication date: 2001
Main Research Area: Technical/natural sciences

Publication information
Journal: I&EC Research
Volume: 40
Issue number: 13
Original language: English
Source: orbit
Source-ID: 40992
Publication: Research - peer-review › Journal article – Annual report year: 2001

Changes in Asphaltene Chemistry and Stability during Hydrotreating

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Andersen, S. I. (Intern), Mejholm, M. (Ekstern), Bartholdy, J. (Ekstern), Lauridsen, R. (Ekstern)
Publication date: 2000

Host publication information
Title of host publication: 4th International Conference on Chemistry in Industry
Main Research Area: Technical/natural sciences
Conference: 4th International Conference on Chemistry in Industry, 01/01/2000
Source: orbit
Source-ID: 209296
Publication: Research - peer-review › Article in proceedings – Annual report year: 2000
Compositional Analysis of North Sea Oils

The molar fluid composition of either the reservoir fluid or the well stream is determined by combining the true boiling point (TBP) distillation data with gas chromatographic (GC) analysis of the light ends. For the purpose of thermodynamic simulation of phase behavior of petroleum reservoir fluids, in addition to the compositional data, physical properties of the pseudo fractions, i.e., density and molecular weight are required. A major drawback of the TBP distillation is the fact that the fractions contain typically 20 - 30% of the material outside the defined boiling range. Another significant issue is the use of generalized density and molecular weight data in the absence of experimentally determined values. This can introduce major inaccuracies in the phase behavior calculations because the generalized value of density and molecular weight significantly differ in each oil based on the paraffin-naphthene-aromatic distribution and its geographic origin.

In this work we have performed the true TBP distillation of 7 stabilized North Sea oil samples. All the oils were distilled from carbon number 6 to 19 and the distillation was terminated at C20+, which was termed as the residue. We have performed analysis of the C10 fraction of each oil by gas chromatography. Subsequently, the specific gravity and molecular weights of the TBP fractions were determined and compared with the generalized values, which indicated major differences. In addition, the superiority of the PVT calculations for a volatile oil and a gas condensate using the experimentally determined specific gravity and molecular weight of the pseudo fractions against the generalized properties is also demonstrated.
Crude Oil Model Emulsion Characterised by means of Near Infrared Spectroscopy and Multivariate Techniques

Water-in-oil emulsions are investigated by means of multivariate analysis of near infrared (NIR) spectroscopic profiles in the range 1100 - 2250 nm. The oil phase is a paraffin-diluted crude oil from the Norwegian Continental Shelf. The influence of water absorption and light scattering of the water droplets are shown to be strong. Despite the strong influence of the water phase, the NIR technique is still capable of predicting the composition of the investigated oil phase.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Kallevik, H. (Ekstern), Hansen, S. B. (Intern), Sæther, Ø. (Ekstern), Sjöblom, J. (Ekstern), Kvalheim, O. M. (Ekstern)
Pages: 245-262
Publication date: 2000
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Disperstion Science and Technology
Volume: 21
Issue number: 3
ISSN (Print): 0193-2691
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 0.435 SNIP 0.663 CiteScore 1.4
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.339 SNIP 0.652 CiteScore 0.98
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.304 SNIP 0.52 CiteScore 0.83
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.302 SNIP 0.486 CiteScore 0.77
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
Dielectric Studies of Asphaltenes in Toluene Solutions

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Pedersen, C. (Intern), Andersen, S. I. (Intern)
Publication date: 2000

Host publication information
Title of host publication: 2nd International Conference on Petroleum and Gas Phase Behaviour
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 209294
Publication: Research - peer-review › Article in proceedings – Annual report year: 2000

Effect of Low Permeable Porous Media on Behavior of Gas Condensate

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Shapiro, A. (Intern), Potsch, K. (Ekstern), Kristensen, J. G. (Intern), Stenby, E. H. (Intern)
Publication date: 2000
Main Research Area: Technical/natural sciences

Publication information
Bibliographical note
Presented at the SPE European Petroleum Conference in Paris, France, October, 2000
Source: orbit
Source-ID: 209289
Publication: Research - peer-review › Journal article – Annual report year: 2000
Original language: English
Effects of Numerical Dispersion in FD Simulation of 1D Gas Injection Problems

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Jessen, K. (Ekstern), Stenby, E. H. (Intern)
Publication date: 2000
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 209292
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2000

Estimation of Solubility Parameters of Complex Crude Oil Mixtures Using Sound Velocity

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Pedersen, C. (Intern), Andersen, S. I. (Intern)
Publication date: 2000

Host publication information
Title of host publication: 2nd International Conference on Petroleum and Gas Phase Behaviour
Main Research Area: Technical/natural sciences
Conference: 2nd International Conference on Petroleum and Gas Phase Behaviour, 01/01/2000
Source: orbit
Source-ID: 209295
Publication: Research - peer-review › Article in proceedings – Annual report year: 2000

Heat Treatment in the Manufacture of Pitch Produced from Blends of Tars of Petroleum and Coal Origin

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Hansen, B. E. (Ekstern), Malmros, O. (Ekstern), Turner, N. R. (Ekstern), Stenby, E. H. (Intern), Andersen, S. I. (Intern)
Publication date: 2000
Event: Abstract from EUROCARBON 2000, 1st World Conference on Carbon, .
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 209286
Publication: Research › Conference abstract for conference – Annual report year: 2000

Including Capillary Pressure in Simulations of Steady State Relative Permeability Experiments

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Phase Equilibria and Separation Processes, Center for Energy Resources Engineering
Authors: Poulsen, S. (Intern), Skauge, T. (Ekstern), Dyrhol, S. O. (Ekstern), Stenby, E. H. (Intern), Skauge, A. (Ekstern)
Publication date: 2000

Host publication information
Title of host publication: SCA 2000-14
Main Research Area: Technical/natural sciences
Conference: the 2000 International Symposium on the Society of Core Analysts, 01/01/2000
Source: orbit
Source-ID: 209310
Publication: Research - peer-review › Article in proceedings – Annual report year: 2001
Isothermal Gravitational Segregation: Algorithms and Specifications

New algorithms for calculating the isothermal equilibrium state of reservoir fluids under the influence of gravity are presented. Two types of specifications are considered: the specification of pressure and composition at a reference depth; and the specification of the total overall content of the reservoir, along with the reservoir geometry. It is shown how both types of calculations can be performed in an efficient and robust manner using volume-based thermodynamics. The new method makes it possible to evaluate the influence of reservoir geometry and gravity segregation on the hydrocarbon reserves. (C) 2000 Elsevier Science B.V. All rights reserved.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Phase Equilibria and Separation Processes, Center for Energy Resources Engineering
Authors: Halldórsson, S. (Intern), Stenby, E. H. (Intern)
Pages: 175-183
Publication date: 2000
Main Research Area: Technical/natural sciences

Publication information
Journal: Fluid Phase Equilibria
Volume: 175
Issue number: 1-2
ISSN (Print): 0378-3812
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 2.33 SJR 0.869 SNIP 1.155
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.874 SNIP 0.998 CiteScore 1.99
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 0.982 SNIP 1.248 CiteScore 2.28
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.007 SNIP 1.274 CiteScore 2.31
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.152 SNIP 1.286 CiteScore 2.31
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.034 SNIP 1.234 CiteScore 2.26
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 0.986 SNIP 1.317
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.133 SNIP 1.164
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.227 SNIP 1.09
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.031 SNIP 1.151
Low Temperature Treatment of Petroleum Tar in the Production of Anode Binder Pitch

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Hansen, B. E. (Ekstern), Malmros, O. (Ekstern), Turner, N. R. (Ekstern), Stenby, E. H. (Intern), Andersen, S. I. (Intern)
Publication date: 2000
Event: Abstract from 2nd International Conference on Petroleum and Gas Phase Behaviour, Copenhagen, Denmark.
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 209293
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2000

Measurement of Phase Boundaries of Hydrocarbon Mixtures Using Fiber Optical Detection Techniques

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Phase Equilibria and Separation Processes, Center for Energy Resources Engineering
Authors: Dandekar, A. (Intern), Stenby, E. H. (Intern)
Pages: 2586-2591
Publication date: 2000
Main Research Area: Technical/natural sciences

Publication information
Journal: Industrial & Engineering Chemistry Research
Volume: 39
Issue number: 7
ISSN (Print): 0888-5885
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Modeling and Simulation of Nitrogen Injection in a Naturally Fractured Reservoir

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Phase Equilibria and Separation Processes, Center for Energy Resources Engineering
Authors: Jákupsstovu, S. I. (Intern), Quiñones-Cisneros, S. E. (Ekstern), Stenby, E. H. (Intern)
Publication date: 2000
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 209280
Publication: Research › Conference abstract for conference – Annual report year: 2000

Modeling of Characterized Oils Viscosity with the One Parameter Friction Theory Models

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Quiñones-Cisneros, S. E. (Ekstern), Zéberg-Mikkelsen, C. K. (Ekstern), Stenby, E. H. (Intern)
Publication date: 2000
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 209290
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2000

Models for Surfactant Systems

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Phase Equilibria and Separation Processes, Center for Energy Resources Engineering
Authors: Cheng, H. (Intern), Kontogeorgis, G. (Intern), Stenby, E. H. (Intern)
Publication date: 2000

Publication information
Publisher: Internal Report
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 209279
Publication: Research › Report – Annual report year: 2000

Rate Effects on Centrifuge Drainage Relative Permeability

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Skauge, A. (Ekstern), Poulsen, S. (Intern)
Pages: 457-467
Publication date: 2000
Main Research Area: Technical/natural sciences

Publication information
Journal: SPE journal
Volume: 63145
Issue number: Vol.SIGMA
ISSN (Print): 1086-055X
Ratings:
BFI (2018): BFI-level 1
Recommended Viscosity Data and Models: n-Alkanes

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Phase Equilibria and Separation Processes, Center for Energy Resources Engineering
Authors: Zeberg-Mikkelsen, C. K. (Intern), Cisneros, S. (Intern), Stenby, E. H. (Intern)
Publication date: 2000
Solid Organic Deposition During Gas Injection Studies
Recently a series of first contact miscibility (swelling) experiments have been performed on undersaturated light and heavy oils using LPG rich and methane rich injection gases, in which solid organic deposition was observed. A compositional gradient in the oils during the gas injection process was also evident as oil fractions expelled from the top to bottom of the PVT cell were observed to vary in density, molecular weight, as well as darkness of color. The change in stability of the oil samples before and after the contact with gas was analyzed using flocculation threshold titration. The asphaltene content of the different oil samples were determined by the TP 143 method. The standard asphaltenes and the solid organic deposit recovered from the swelling tests were analyzed using FTIR, HPLC-SEC and H-1 NMR. The aim of these analyses is to reveal the molecular nature of the deposits formed during the gas injection process in comparison with the standard asphaltenes in order to understand the mechanisms involved in asphaltene deposition.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Phase Equilibria and Separation Processes, Center for Energy Resources Engineering
Authors: Dandekar, A. Y. (Ekstern), Andersen, S. I. (Intern), Stenby, E. H. (Intern)
Pages: 1209-1229
Publication date: 2000
Main Research Area: Technical/natural sciences

Publication information
Journal: Petroleum Science and Technology
Volume: 18
Issue number: 9-10
ISSN (Print): 1091-6466
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 0.285 SNIP 0.508 CiteScore 0.6
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.265 SNIP 0.584 CiteScore 0.48
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.296 SNIP 0.774 CiteScore 0.4
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.411 SNIP 0.851 CiteScore 0.48
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.271 SNIP 0.565 CiteScore 0.38
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.322 SNIP 0.637 CiteScore 0.5
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.27 SNIP 0.439
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.362 SNIP 0.544
BFI (2008): BFI-level 1
The Mystery of the Van der Waals Equation

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Kontogeorgis, G. (Intern), Coutsikos, P. H. (Ekstern)
Publication date: 2000

Publication information
Publisher: Technical University of Denmark, Department of Chemical Engineering
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 209285
Publication: Research › Report – Annual report year: 2000

Thermodynamics, Impurities, and Kinetics in the Process of Sucrose Crystallisation

General information
Three-Dimensional Compositional Simulation: Streamline Methods and Analytical Solutions for One-Dimensional Flow

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Ermakov, P. (Ekstern), Jessen, K. (Intern), Zhu, J. (Ekstern), Orr Jr., F. M. (Ekstern)
Publication date: 2000
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 209291
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2000

Speeding up the Two-Phase PT-flash, with Applications for Calculation of Miscible Displacement

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Michelsen, M. L. (Intern)
Pages: 1-12
Publication date: 1998
Main Research Area: Technical/natural sciences

Publication information
Journal: Fluid Phase Equilibria
Volume: 143
Issue number: 1-2
ISSN (Print): 0378-3812
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 2.33 SJR 0.869 SNIP 1.155
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.874 SNIP 0.998 CiteScore 1.99
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 0.982 SNIP 1.248 CiteScore 2.28
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.007 SNIP 1.274 CiteScore 2.31
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.152 SNIP 1.286 CiteScore 2.31
Vapor-Liquid Equilibria by UNIFAC Group Contribution. 5. Revision and Extension

General information
State: Published
Organisations: Department of Chemistry, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Hansen, H. K. (Intern), Rasmussen, P. (Intern), Fredenslund, A. (Ekstern), Schiller, M. (Ekstern), Gmehling, J. (Ekstern)
Pages: 2352-2355
Publication date: 1991
Main Research Area: Technical/natural sciences

Publication information
Journal: Industrial & Engineering Chemistry Research
Volume: 30
Issue number: 10
ISSN (Print): 0888-5885
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering, Technical University of Denmark
Authors: Gmehling, J. (Ekstern), Rasmussen, P. (Intern), Fredenslund, A. (Ekstern)
Pages: 724-734
Publication date: 1980
Main Research Area: Technical/natural sciences

Publication information
Journal: Chemie-Ingenieur-Technik
Volume: 52
Issue number: 9
ISSN (Print): 0009-286X
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 0.355 SNIP 0.596 CiteScore 0.83
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.342 SNIP 0.584 CiteScore 0.69
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.327 SNIP 0.558 CiteScore 0.77
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.288 SNIP 0.504 CiteScore 0.62
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.343 SNIP 0.531 CiteScore 0.55
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.238 SNIP 0.497 CiteScore 0.42
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.21 SNIP 0.344
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.255 SNIP 0.45
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.196 SNIP 0.277
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 0.187 SNIP 0.297
Scopus rating (2006): SJR 0.171 SNIP 0.249
Scopus rating (2005): SJR 0.184 SNIP 0.323
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 0.223 SNIP 0.312
Scopus rating (2003): SJR 0.197 SNIP 0.443
Scopus rating (2002): SJR 0.257 SNIP 0.464
On the Combinatorial Part of the UNIFAC and UNIQUAC Models

The excess Gibbs energy of liquid mixtures may be predicted using group contribution models (e.g. UNIFAC and ASOG), or it may be correlated using molecular models such as UNIQUAC. Group contribution models and the UNIQUAC model contain a combinatorial contribution which accounts for size- and shape-effects and a residual contribution which accounts for interactions among groups or molecules. A new expression for the combinatorial contribution is given which yields much improved predictions of the excess Gibbs energy of systems where the residual contribution may be expected to be zero (e.g., mixtures of aliphatic hydrocarbons). It is shown that it is advantageous to incorporate the new combinational expression into future modifications of the UNIFAC model.

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering, Technical University of Denmark
Authors: Kikic, I. (Ekstern), Alessi, P. (Ekstern), Rasmussen, P. (Intern), Fredenslund, A. (Ekstern)
Publication date: 1980

Publication information
Publisher: Technical University of Denmark, Department of Chemical Engineering
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 262131
Publication: Research › Report – Annual report year: 1980

Journal: Canadian Journal of Chemical Engineering
Volume: 58
Issue number: 2
ISSN (Print): 0008-4034
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.41 SJR 0.504 SNIP 0.805
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.41 SNIP 0.656 CiteScore 1.13
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.504 SNIP 0.815 CiteScore 1.28
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.476 SNIP 0.798 CiteScore 1.16
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.427 SNIP 0.813 CiteScore 0.99
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.429 SNIP 0.692 CiteScore 0.94
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.415 SNIP 0.627
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.365 SNIP 0.68
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.358 SNIP 0.481
Scopus rating (2007): SJR 0.449 SNIP 0.534
Scopus rating (2006): SJR 0.344 SNIP 0.631
Scopus rating (2005): SJR 0.428 SNIP 0.784
Scopus rating (2004): SJR 0.378 SNIP 0.629
Scopus rating (2003): SJR 0.513 SNIP 0.552
Scopus rating (2002): SJR 0.677 SNIP 0.858
Scopus rating (2001): SJR 1.003 SNIP 1.174
Scopus rating (2000): SJR 0.736 SNIP 0.929
Web of Science (2000): Indexed yes
Scopus rating (1999): SJR 0.566 SNIP 0.914
Original language: English
DOIs:
10.1002/cjce.5450580218
Links:
http://www3.interscience.wiley.com/journal/122284698/abstract
Source: orbit
Source-ID: 262126
Publication: Research - peer-review › Journal article – Annual report year: 1980

On the Temperature Dependence of the UNIQUAC/UNIFAC Models
Local composition models for the description of the properties of liquid mixtures do not in general give an accurate representation of excess Gibbs energy and excess enthalpy simultaneously. The introduction of temperature dependent interaction parameters leads to considerable improvements of the simultaneous correlation. The temperature dependent parameters have, however, little physical meaning and very odd results are frequently obtained when the interaction parameters obtained from excess enthalpy information alone are used for the prediction of vapor-liquid equilibria. The UNIQUAC/UNIFAC models are modified in this work by the introduction of a general temperature dependence of the coordination number. The modified UNIQUAC/UNIFAC models are especially suited for the representation of mixtures containing non-associating components. The modified models contain the same number of interaction parameters as the original ones, namely two per binary pair of molecules/groups. The resulting simultaneous representation of excess Gibbs energy and excess enthalpy by means of one unique set of parameters is remarkably successful. One may with very good results predict excess Gibbs energy information from UNIQUAC parameters based on excess enthalpy data, and the prediction of excess enthalpy information from only one isothermal set of vapor-liquid equilibrium data is qualitatively acceptable. A parameter table for the modified UNIFAC model is given for the five main groups: CH2, C = C, ACH, ACCH2 and CH2O.

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering, Technical University of Denmark
Authors: Skjold-Jørgensen, S. (Ekstern), Rasmussen, P. (Intern), Fredenslund, A. (Ekstern)
Pages: 2389-2403
Publication date: 1980
Main Research Area: Technical/natural sciences
Thermodynamic Properties from Corresponding States Theory

A corresponding states approach has been applied to the two-constant equations of state by Wilson, Soave, Peng—Robinson, Hamam et al., Lu et al., Simonet—Behar, and Chaudron et al. in order to obtain the equivalent shape-factor correlations. The correlations derived are compared with the Leach—Leland corresponding-states theory. Different fluid approximations for mixtures have been applied to the various corresponding states approaches. The resulting computation methods have been applied to calculate saturation properties of pure fluids and separation factors in binary mixtures for some fluids commonly encountered in natural gas and petroleum refining operations. Finally it is shown that the binary interaction parameters depend only on the fluid approximation and not on the specific form of the potential.
Thermodynamics, Design, Simulation and Benchmarking of Biofuel Processes

A new framework at DTU contributes to the sustainable development of technologies for green synthetic fuel production from biomass. Thermochemical biomass gasification is carried out, followed by fermentation of the created syngas to biofuels. The ultimate scope is a complete design which will include energy efficient product separation, process analysis and optimization as well as comparison to competitive market Technologies.

In brief, the technological focus and scientific objectives are: 1) Fermentation of syngas to liquid (alcohols) and gaseous (methane) biofuels focusing on applying mixed microbial consortia, 2) Design of novel bioreactors, pressure control and use of suitable surfactants for increasing the gas/liquid mass transfer efficiency, 3) Use of biomimetic membranes and development of diabatic distillation for gentle and cost-efficient purification of liquid biofuels and 4) Development of an optimized process design and comparison with existing Technologies.

The technology to be developed will contribute to a more sustainable society producing energy from non-food related biomass without a catalytic conversion. Today syngas from biomass is used in combined heat and power production (CHP). By merging the CHP production with the fermentation of syngas, the processing of syngas can always follow the optimum path. That is, the final production will be easily diverted to CHP or biofuels satisfying thus the supply and demand of the biomass and energy markets. For example, when the heating demand is high, the syngas will mainly be exploited through CHP but when the heating demand is low, the syngas will be fermented to storable liquid or gaseous biofuels.

Purpose of the project

The task is to process simulate the fermentation technologies of syngas developed in this project. This covers both methanation and liquid fuel production. Simulations will be carried out and compared to other competitive literature methods to benchmark the technologies from a mass, energy, economic and engineering point of view. The designs will likely be carried out with the commercial process simulator Aspen Plus.

Project contents

The core of your project is to develop a thermodynamic model parameter base. Knowledge will be collected from the project platform to model the observed phenomenon. The investigations will include data from literature and includes thermodynamic modeling, possibly supported by experimental work. The knowledge will be applied in software programming and in a more high level process simulation interface to Aspen Plus. The CERE group has a selection of available interfaces which will be exploited as part of this work. The global aim is to perform process simulation of several different syngas fermentation designs and furthermore compare these with the aim of benchmarking the performance of the various technologies towards commercial processes.

Center for Energy Resources Engineering

Department of Chemical and Biochemical Engineering
CERE – Center for Energy Resources Engineering
Period: 01/07/2015 → 30/06/2019
Number of participants: 1
Acronym: Synferon
Project participant:
Fosbøl, Philip Loldrup (Intern)

**Sulphur (SOx) corrosion in large diesel engines**

Project entails experimental and modeling of current densities during corrosion from sulphur as a consequence of the combustion process in large diesel ship engines

Center for Energy Resources Engineering

Department of Chemical and Biochemical Engineering

CERE – Center for Energy Resources Engineering
Period: 01/07/2015 → 01/01/2019
Number of participants: 1
Acronym: SulCor
Number of related Ph.D. students: 1
Project participant:
Fosbøl, Philip Loldrup (Intern)

**Temperature and poroelasticity of sedimentary rocks**

The project is centered on development of rock mechanics related to high pressure and high temperature (HP/HT) conditions in the subsurface. The issue will be addressed experimentally and theoretically including numerical modeling.

Hydrocarbon reservoirs deeply buried under the central North Sea are not only subjected to high temperatures and a stress-field corresponding to depths of 5 km or more. They are also situated at a depth with high regional overpressure. This gives rise to three key challenges, which apply not only in the North Sea but world-wide: 1. Safety during drilling operations due to the extreme pressure and stresses. 2. Well life – the danger of well collapse under extreme stress conditions. 3. Controlling the drilling operation due to narrow drilling windows, in particular during infill drilling. This latter challenge must be met in order to maximize recovery.

In order to address these challenges we must develop methods to determine how the effective stress field responds to changes in pore pressure under these extreme conditions. The effective stress field is primarily a function of the weight of the overburden and how much of the load, the fluids in the rock carry. It also depends on the elastic properties of the rock at a given depth.

Supervisor: Prof. Ida Lykke Fabricius, ilfa@byg.dtu.dk

co-supervisor: Ass. Prof. Katrine Alling Andreassen, kall@byg.dtu.dk

Department of Civil Engineering
Center for Energy Resources Engineering
Department of Chemical and Biochemical Engineering
CERE – Center for Energy Resources Engineering

Department of Geology and Geotechnical Engineering
Period: 01/08/2014 → 01/08/2017
Number of participants: 1
Project participant:
Orlander, Tobias (Intern)

**Relations**

Related projects:

Heat Storage in Hot Aquifers
Effective high-resolution Geological Modeling

It is the vision of this project to build an user friendly expert system, which is able to combine very large amounts of hard geological, geochemical and geophysical data with geological expert knowledge and information about an area. This approach in building geological models (Smart Interpretation) will facilitate fast, consistent, accurate and reliable modelling of very large areas. It will also facilitate construction of models with very high resolution, (High Definition Models) as the system will "learn" the geology of an area directly from a geological interpretation made by a geological expert. The system can then be used in another similar area by an untrained geologist to build a geological model, guided by the experienced geologists way of interpolation, as quantified by the expert system.

Center for Energy Resources Engineering
Mathematical and Computational Geoscience
Period: 01/09/2013 → 01/09/2016
Number of participants: 2
Acronym: ERGO
Project ID: 113-2013-1
Project Manager, organisational: Mosegaard, Klaus (Intern)
Project Manager, academic: Hansen, Thomas Mejer (Intern)

Wood Coatings
Center for Energy Resources Engineering
Department of Chemical and Biochemical Engineering
CERE – Center for Energy Resources Engineering
Period: 01/05/2012 → 30/11/2016
Number of participants: 1
Project ID: 50902
Project Manager, academic: Kontogeorgis, Georgios (Intern)

CHIGP Petrobras
Center for Energy Resources Engineering
Department of Chemical and Biochemical Engineering
CERE – Center for Energy Resources Engineering
Period: 01/02/2012 → 31/12/2014
Number of participants: 2
Project ID: 50894
Other:
Biede, Anne Louise (Intern)
Project Manager, organisational: Kontogeorgis, Georgios (Intern)

CHIGP Petrobras
Funded by Petrobras
Center for Energy Resources Engineering
Department of Chemical and Biochemical Engineering
CERE – Center for Energy Resources Engineering
CO2 Kompression
Funded by Lloyds Register
Center for Energy Resources Engineering
Department of Chemical and Biochemical Engineering
CERE – Center for Energy Resources Engineering
Period: 01/02/2012 → 31/12/2012
Number of participants: 1
Project ID: 50894
Project Manager, academic:
Kontogeorgis, Georgios (Intern)

Development of Non Destructive Methods
Funded by "Fonden for ikke-destruktiv prøvning"
Center for Energy Resources Engineering
Department of Chemical and Biochemical Engineering
CERE – Center for Energy Resources Engineering
Period: 01/02/2012 → 31/03/2016
Number of participants: 1
Project ID: 50893
Project Manager, academic:
Fosbøl, Philip Loldrup (Intern)

Heat Storage in Hot Aquifers
Department of Civil Engineering
Section for Geotechnics and Geology
Center for Energy Resources Engineering
Department of Informatics and Mathematical Modeling
Scientific Computing
Period: 01/01/2012 → 28/02/2015
Number of participants: 3
Number of related Ph.D. students: 1
Project participant:
Rosenbrand, Esther (Intern)
Mosegaard, Klaus (Intern)
Project Manager, academic:
Fabricius, Ida Lykke (Intern)

CO2 Hydrates-Challenges and Possibilities
While great efforts are undertaken in oil and gas exploration to inhibit the formation of hydrates which may lead to production stops, it has been suggested that in relation to carbon capture, hydrate formation should instead be actively stimulated. A joint CERE/Ecole des Mines (France) project addresses both challenges and possibilities.

Funded by FIST
Center for Energy Resources Engineering
Department of Chemical and Biochemical Engineering

CERE – Center for Energy Resources Engineering
Period: 08/11/2011 → 30/06/2014
Number of participants: 1
Project ID: 50868
Project Manager, academic: Kontogeorgis, Georgios (Intern)

Otto Mønsted
Funded by Otto Mønsted’s Fond
Center for Energy Resources Engineering

Department of Chemical and Biochemical Engineering
CERE – Center for Energy Resources Engineering
Period: 01/10/2011 → 31/12/2012
Number of participants: 1
Project ID: 50863
Project Manager, academic: von Solms, Nicolas (Intern)

Heat Storage in Hot aquifers
Department of Civil Engineering
Section for Geotechnics and Geology
Center for Energy Resources Engineering
Department of Environmental Engineering
Period: 01/06/2011 → 31/05/2014
Number of participants: 3
Phd Student: Rosenbrand, Esther (Intern)
Supervisor: Kjøller, Claus (Intern)
Main Supervisor: Fabricius, Ida Lykke (Intern)

Smart Water
Water flooding is a standard method to extract extra oil from mature fields. International research suggests that the impact may be increased by modifying salinity or other features of the injected water. Involving industrial partners the Smart Water project led by CERE is focussed on both theoretical understanding and practical applications.

Funded by Energistyrelsen, DONG Energy and Maersk Oil
Center for Energy Resources Engineering
Department of Chemistry
Department of Civil Engineering
Section for Geotechnics and Geology
Period: 01/06/2011 → 30/09/2014
Number of participants: 2
Project ID: 50845
Project Manager, academic: Stenby, Erling Halfdan (Intern)
Project Coordinator: Fabricius, Ida Lykke (Intern)
BioRec
BioRec is a Danish research program involving several industrial and research partners. The program is focused on both Microbial Enhanced Oil Recovery (MEOR) and enzymatic enhanced oil recovery while also looking into innovative use of biotechnology in relation to prevention of corrosion and gas hydrate formation. The program is led by CERE.

Funded by HTF
Center for Energy Resources Engineering
Department of Chemistry
Period: 15/03/2011 → 30/09/2015
Number of participants: 1
Project Manager, academic:
Stenby, Erling Halfdan (Intern)

CHIGP-GERG
The water content of natural gas often poses problems during production, transmission and distribution. Use of production chemicals like glycols and alcohols add to complexity. CERE is the academic partner of a collaborative R&D project on the subject initiated by The European Gas Research Group (GERG).

Funded by Dansk Gæsteknisk Center
DOC 09/03719
Center for Energy Resources Engineering
Department of Chemical and Biochemical Engineering
CERE – Center for Energy Resources Engineering
Period: 01/03/2011 → 01/07/2014
Number of participants: 1
Project Manager, academic:
Kontogeorgis, Georgios (Intern)

Heat Storage in Hot Aquifers
In this project, we will develop new technology to improve planning of energy storage in geothermal reservoirs through high-quality experiments and modelling. Geothermal reservoirs have high temperature, so energy may be stored in these geological layers with minimal heat loss. The technology will be based on a multidisciplinary approach combining small scale geochemistry/rock physics with large scale seismic inversion and history matching of production data. The focus will be on Danish geothermal reservoirs, because heat storage is likely to be the missing link in planning sustainable energy production in Denmark, where several sources of energy should interplay. Energy sources as waste incineration and wind are not controlled by immediate energy demands. By storing energy at low heat loss in hot aquifers, we obtain an effective interplay between different sources of energy. Thereby, the degree of coverage with sustainable energy can increase at an acceptable cost. It is the right time to do this, because geothermal plants are presently being installed in Denmark. Thus, the cost of establishing heat storage in geothermal reservoirs is relatively small. The imminent question with respect to establishing heat storage in geothermal reservoirs is how the reservoirs will react to the introduction of water with a higher temperature than the natural as compared to effects of injecting cold water: How will the reservoir rock react chemically and mechanically, how will the heat and fluid distribute in the reservoir, what is the energy loss related to this storage method, and how will a potential change in water chemistry influence the operation abilities of the geothermal plant? We will evaluate the technology in an international context by collaborating with researchers working with geothermal reservoirs in other European countries.

Center for Energy Resources Engineering
Center
Department of Civil Engineering
Department of Informatics and Mathematical Modeling
De Nationale Geologiske Undersøgelser for Danmark og Grønland
BRGM
Vilnius University
Eidgenössische Technische Hochschule
DONG Energy A/S
Senderborg Fjernvarme A.m.b.a.
Københavns Energi A/S
CTR I/S

VEKS
Period: 01/03/2011 → 28/02/2015
Number of participants: 17
Acronym: HeHo
Project ID: 11/00125
Contact person:
Azaroual, Mohamed (Ekstern)
Sliaupa, Saulius (Ekstern)
Khan, Amir (Ekstern)
Magtengaard, Jesper (Ekstern)
Moe, Steffen (Ekstern)
Foged, Magnus (Ekstern)
Elleris, Jan (Ekstern)
Andersen, Flemming (Ekstern)
Project participant:
Rosenbrand, Esther (Intern)
Holmstykke, Hanne Dahl (Ekstern)
Lopez, Simon (Ekstern)
Bickauskas, Giedrius (Ekstern)
Mahler, Allan (Ekstern)
Ragen, Birte (Ekstern)
Project Manager, organisational:
Fabricius, Ida Lykke (Intern)
Mosegaard, Klaus (Intern)
Kjøller, Claus (Ekstern)

Financing sources
Source: Forskningsrådene - Andre
Name of research programme: Forskningsrådene - Andre
Amount: 5,658,000.00 Danish Kroner

Heat Storage in Hot Aquifers
Department of Civil Engineering
Section for Geotechnics and Geology
Center for Energy Resources Engineering
Department of Informatics and Mathematical Modeling
Scientific Computing
Department of Environmental Engineering
Period: 01/03/2011 → 28/02/2012
Number of participants: 4
Project participant:
Mosegaard, Klaus (Intern)
Kjøller, Claus (Intern)
Phd Student:
Rosenbrand, Esther (Intern)
**Reson**
Funded by Højteknologifonden  
DOC 11/03305  
Center for Energy Resources Engineering  
Department of Chemical and Biochemical Engineering  
CERE – Center for Energy Ressources Engineering  
Period: 01/03/2011 → 31/12/2014  
Number of participants: 1  
Project ID: 50826  
Project Manager, academic:  
Kontogeorgis, Georgios (Intern)  

**Disc. Meeting, løbende**
Funded by: Deltagerbetalning  
Center for Energy Resources Engineering  
Department of Chemistry  
Period: 01/02/2011 → 31/12/2020  
Number of participants: 1  
Project ID: 50807  
Project Manager, academic:  
Stenby, Erling Halfdan (Intern)  

**Ph.D. Advanced Course on Thermodynamic Models: Fundamentals & Computational Aspects**
Funded by: Deltagerbetalning  
Center for Energy Resources Engineering  
Department of Chemical and Biochemical Engineering  
CERE – Center for Energy Ressources Engineering  
Period: 01/02/2011 → 30/11/2011  
Number of participants: 1  
Acronym: Ph.D. Kursus MLM  
Project Manager, academic:  
Kontogeorgis, Georgios (Intern)  

**Gas Hydrate Inhibition with Ice-Structuring Proteins**
Large quantities of gas hydrate inhibitors, primarily methanol and glycol, secure oil recovery under cold and high-pressure conditions. The present CERE project follows up on previous research which suggested that proteins found in bark beetle, meal worm and Arctic fish species might be able to do the job more efficiently.  
Funded by FIST  
DOC 10/01685  
Center for Energy Resources Engineering  
Department of Chemical and Biochemical Engineering  
CERE – Center for Energy Ressources Engineering  
Period: 01/12/2010 → 30/05/2014  
Number of participants: 1  
Project ID: 50805  
Project Manager, academic:
von Solms, Nicolas (Intern)

**CLEO Forskningsprojekt**
Funded by TNO
DOC 08/03100

Under lukning

Center for Energy Resources Engineering
Department of Chemical and Biochemical Engineering
CERE – Center for Energy Resources Engineering
Period: 01/05/2010 → 31/12/2010
Number of participants: 1
Project ID: 50766
Project Manager, academic:
Thomsen, Kaj (Intern)

**CERE Administration**
Center for Energy Resources Engineering
Department of Chemistry
Period: 01/01/2010 → 10/10/2020
Number of participants: 1
Project ID: 50678
Project participant:
Stenby, Erling Halfdan (Intern)

**CHIGP DONG**
Funded by DONG Energy
DOC 10/00681

Center for Energy Resources Engineering
Department of Chemical and Biochemical Engineering
CERE – Center for Energy Resources Engineering
Period: 01/01/2010 → 31/03/2013
Number of participants: 1
Project Manager, academic:
Kontogeorgis, Georgios (Intern)

**Innovative CO2 Capture**
Funded by NTNU/EU 7
DOC 10/01054

Center for Energy Resources Engineering
Department of Chemical and Biochemical Engineering
CERE – Center for Energy Resources Engineering
Period: 01/01/2010 → 30/06/2014
Number of participants: 1
Acronym: EU ICAP
Project ID: 50751
Project Manager, academic:
von Solms, Nicolas (Intern)

**Relations**
Publications:
Freezing Point Depressions of Phase Change CO2 Solvents
Heat of Absorption of CO2 in Phase Change Solvents: 2-(Diethylamino)ethanol and 3-(Methylamino)propylamine

**Measurements and Modeling of Thermodynamics of Organic Sulfur Species in Hydrocarbons and Pure Water**
Funded by FIST
DOC 09/01183

Center for Energy Resources Engineering
Department of Chemical and Biochemical Engineering
CERE – Center for Energy Resources Engineering
Period: 01/01/2010 → 31/12/2012
Number of participants: 1
Acronym: CHIGP Sulfur
Project ID: 50707
Project Manager, academic:
Awan, Javeed (Intern)

**Complex Phase Behavior and Modeling of Multicomponent Mixtures Containing CO2**
Funded by Gassco
DOC 09/02510

Center for Energy Resources Engineering
Department of Chemical and Biochemical Engineering
CERE – Center for Energy Resources Engineering
Period: 01/09/2009 → 01/06/2012
Number of participants: 1
Acronym: CHIGP Gassco
Project ID: 50660
Project Manager, academic:
Kontogeorgis, Georgios (Intern)

**ParPor - Particles in Pores. Stochastic Modeling of Polydisperse Transport**
Particle transport in porous media takes place in a range of contexts, i.e. industrial filtration, waste water treatment, mass transfer in human tissues, mud filtration around oil wells and others. Based on a stochastic approach the CERE project develops software for practical use in modeling of flows of suspensions in porous media.

Funded by FIST
DOC 09/01186

Center for Energy Resources Engineering
Department of Chemical and Biochemical Engineering
CERE – Center for Energy Resources Engineering
Period: 01/09/2009 → 31/08/2012
Number of participants: 1
Acronym: ParPor
Project ID: 50711
Project Manager, academic:
Shapiro, Alexander (Intern)

**Ionic Liquids for CO2 Capture**
Funded by FIST, DONG Energy and Mærsk Oil
DOC 09/00224

Under lukning
As easily accessible oil reserves are becoming scarcer, the need for new approaches in Enhanced Oil Recovery (EOR) is growing. The Advanced Oil Recovery Methods (ADORE) project led by CERE encompasses a range of research disciplines with the objective of adding to recoverable hydrocarbon reserves via novel or improved EOR methodologies.

Funded by FIST

Center for Energy Resources Engineering
Raman spectroscopy by use of UltraViolet Radiation : A new useful way to avoid fluorescence

Fluorescence has been a persistent problem in Raman spectroscopy. To avoid the problems a way to seems to have opened now: Excitation with deeply ultraviolet light. "Fluorescence does not appear to exist if the exciting light has a wavelength shorter than 260 nm" [cit. S. A. Asher]. Affordable pulsed deep-UV lasers have recently been introduced to the market by a company "Photon Systems" in California. So-called HeAg og NeCu hollow-cathode lasers during operation create a metal vapor mixed with an inactive rare gas by a process reminding of sputtering. The lasers emit quasi-continuous laser light in the deep UV-range, with wavelengths of 224 nm (for silver) and 248 nm (for copper). During operation they require little electrical power and no water cooling. New instrument needed. We apply for a dedicated UV Raman-spectrometer with quartz optics, UV grating and detectors, and the necessary helping utensils. One important new aspect of the method is to introduce optical fibers, so that the optics can be totally encapsulated to avoid any deep UV radiation damage to objects and persons in the neighbourhood. UV-Raman spectroscopy will have many future applications. We will try the technique in three limited, well-defined research fields with a high content of new and innovative ideas. Hence, we want a new laser to abate fluorescence. We would like to use the new system in this way: 1) Characterisation of new waveguides by use of hollow microstructured crystal fibers. It ranges from analysis of Ge-nano-clusters embedded in silica-on-silicon planar waveguides to chemical and biological molecular identification. Samples will be prepared and investigated to find better methods to prepare silica materials with enhanced third order nonlinearity. Size
and distribution of the nano-clusters are important parameters. In contrast to other methods, UV-Raman spectroscopy needs no specimen preparation and should be a non-destructive, efficient method to find the size distribution of even very small nano-clusters. The UV Raman will be tried using hollow micro-structured optical fibers. Such air-hole fibers should enable easy and safe UV spectroscopy. This entirely new concept will be tried as well as fibers designed such that the air holes are used both for light guiding and at the same time as pipettes for a chemical solution (like gasoline/methanol mixtures) that one wants to analyse (co-work with COM-center). 2) Characterisation of fluorescing crude oil mixtures to help easy production and less pollution. Polycyclic aromatic hydrocarbons (PAHs) are highly intensive and characteristic Raman scatterers. Even small amounts (ppm to ppb scale or less) should be detectable (co-work with IVC-SEP-center). 3) Characterisation of biological and consumer samples, where fluorescence is a problem. Organic molecules, e.g. proteins, nucleic acids (DNA), hormones, phthalates and pigments in the household and other environments should exhibit Raman and resonance Raman spectra with a lot of information on structure and function if only the fluorescence could be avoided. We will try this by a study of insulin in living tissue (distribution, structure and other characterisations). Also we will start on the obvious project of cancer cell characterisation (a co-work with the QUP-center). 4) We are also studying pigments and objects from the Ny Carlsberg Glyptotek. The intention is to set the UV Raman instrument up, and then carry out the subprojects 1) - 4) simultaneously. The ph.d. project will have the complete set of subprojects as its objective, but parts of the work are to be done even without a ph.d.-salary.

Department of Chemistry
Department of Chemical and Biochemical Engineering
Center for Energy Resources Engineering
Period: 01/01/2006 → 01/01/2009
Number of participants: 1
Acronym: UVRS
Project Manager, organisational: Søtofte, Inger (Intern)

Financing sources
Source: Uddannelse, udenlandske offentlige og private
Name of research programme: Uddannelse, udenlandske offentlige og private
Amount: 10,000.00 Danish Kroner
Project

Petrochallenge – a Competition for High Schools
By combining fun and education, the international PetroChallenge competition encourages high school students in a growing number of countries to take interest in energy resources engineering. CERE has been organizing the national branch of the annual competition since its introduction in Denmark in 2005.

Funded by DONG Energy and Maersk Oil
Center for Energy Resources Engineering
Department of Chemistry
Period: 17/12/2004 → 31/12/2020
Number of participants: 1
Project ID: 50365
Project Manager, academic: Stenby, Erling Halfdan (Intern)

CHIGP BP
Funded by BP
Center for Energy Resources Engineering
Department of Chemical and Biochemical Engineering
CERE – Center for Energy Ressources Engineering
Period: 05/11/2004 → 31/12/2013
Number of participants: 1
Project ID: 50357
Project Manager, academic: Kontogeorgis, Georgios (Intern)
**Priorities** - Improved Oil Recovery and Productivity from Lower Cretaceous Carbonates

Joint project between IVC-SEP and the Geological Survey of Denmark, Sponsored by the EFP programs EFP-97 and EFP-99.

Department of Chemical and Biochemical Engineering

Center for Energy Resources Engineering

Period: 01/03/1999 → 31/12/2002

Number of participants: 1

Project Manager, academic:

Jørgensen, Marianne (Intern)

Project

**Diffusion in liners in offshore flexible pipes**

Flexible high pressure pipes are increasingly used in marine environments for the transportation of well fluids. A flexible pipe consists typically of an inner and outer polymer tube (inner lining and outer sheath), with a number of helically wound steel armour profiles in between. The purpose of the inner lining is to provide the pipe with a leak tight barrier against the transported fluids whereas the outer sheath protects the armour wires from the external environment, e.g. the sea water. A supporting metallic carcass may be applied internally in the pipe bore to increase the collapse strength of the inner lining.

The objective of this project is to establish a reliable method for calculating the resulting concentrations of methane, carbon dioxide and hydrogen sulphide in the annulus of flexible high pressure pipes when subjected to varying operational conditions.

Department of Chemical and Biochemical Engineering

Center for Energy Resources Engineering

NKT Research & Innovation A/S

NKT Flexibles A/S

Period: 01/01/1999 → 31/12/2001

Number of participants: 5

Project participant:

Hassager, Ole (Intern)

Kristensen, Susanne Brogaard (Intern)

Marcher, Bjørn (Ekstern)

Nielsen, Niels Risshøj (Ekstern)

Project Manager, organisational:

Szabo, Peter (Intern)

**Financing sources**

Source: Unknown

Name of research programme: Ukendt

Amount: 1,200,000.00 Danish Kroner

**IVC-SEP Program Package (B.1)**

During the last decades, a great number of programs has been developed for the analysis of phase equilibria and the design of separation processes of simple and complex mixtures. The IVC-SEP has contributed with many of these...
programs which are used in this and other institutions around the world. In order to continue with this contribution, we are working on two main objectives: the development of a new user interface and the creation of a standard subroutine library. The user interface will integrate the majority of programs and databases within the IVC-SEP in a user friendly framework. The library of standard subroutines will simplify the reuse of our programs by internal and external users.

Department of Chemical and Biochemical Engineering

Center for Energy Resources Engineering

Period: 01/01/1998 → 31/12/1999
Number of participants: 1

Project Manager, organisational:
Pretel, Eduardo (Intern)

Raman Spectroscopy Analysis of Phase Equilibria

Phase Equilibria in multicomponent systems, e.g. in fuels, oil and gasses, are studied by Raman and IR spectroscopy. The project is a ph.d. project for Susanne Brunsgaard Hansen, supported by The National Oil and Gas Company of Denmark, The Nordic Energy Research Program and The Danish Technical Research Council.

Department of Chemistry
Department of Chemical and Biochemical Engineering

Center for Energy Resources Engineering

DONG Energy A/S

Nordiske Energiforskningsprogram

Period: 01/07/1997 → 30/01/2001
Number of participants: 3

Project participant:
Hansen, Susanne Brunsgaard (Intern)
Stenby, Erling Halfdan (Intern)

Project Manager, organisational:
Berg, Rolf W. (Intern)

Financing sources

Source: Unknown
Name of research programme: Ubekndt
Amount: 648,000.00 Danish Kroner
Source: Unknown
Name of research programme: Ubekndt
Amount: 274,485.00 Danish Kroner
Source: Unknown
Name of research programme: Ubekndt
Amount: 100,000.00 Danish Kroner
Source: Unknown
Name of research programme: Ubekndt
Amount: 150,000.00 Danish Kroner

Simulation of phase equilibrium and separation processes

The purpose of the project, which is conducted within the IVC-SEP centre, is to develop efficient and robust algorithms for the simulation of phase equilibrium and separation processes. The project also deals with the development and implementation of models for calculation of phase equilibrium and the development of computational tools for this purpose. Algorithms from the Institute are today used worldwide, in particular in the petroleum industry. Recent efforts are concentrated on complex equilibria, as e.g. the treatment of 3-phase equilibria in oil mixtures containing water and hydrate inhibitors, and on developing procedures for cases where the computational speed is all-important, such as flow- and reservoir simulators.

Department of Chemical and Biochemical Engineering

Center for Energy Resources Engineering

Period: 01/01/1980 → 01/01/1981
Number of participants: 1

Project Manager, organisational:
Activities:

**Emulsion Formation for EOR Applications**
Period: 14 Nov 2017 → 15 Nov 2017
Muhammad Waseem Arshad (Speaker)
Department of Chemical and Biochemical Engineering
CERE – Center for Energy Ressources Engineering
Center for Energy Resources Engineering

Description
DHRTC Technology Conference 2017
14-15 November, Kolding, Denmark
Documents:
Final-Programme

**Related external organisation**
Danish Hydrocarbon Research and Technology Centre
Denmark
Activity: Talks and presentations › Conference presentations

**Induration and Biot's Coefficient of Palaeogene Limestone**
Period: 9 Jul 2017 → 13 Jul 2017
Katrine Alling Andreassen (Speaker)
Department of Civil Engineering
Section for Geotechnics and Geology
Center for Energy Resources Engineering
Degree of recognition: International

Related event
6th Biot Conference on Poromechanics
09/07/2017 → 13/07/2017
Paris, France
Activity: Talks and presentations › Conference presentations

**A new association scheme for mono-ethylene glycol within Cubic-Plus-Association equation of state**
Period: 19 May 2017
Francois Kruger (Guest lecturer)
Center for Energy Resources Engineering
Department of Chemical and Biochemical Engineering
CERE – Center for Energy Ressources Engineering

Description
Presentation and poster detailing work on newly proposed association schemes for MEG, along with uncertainty analysis for the parameterization
Degree of recognition: International
Documents:
ESAT 2017: Uncertainty Analysis for the Parameterization of Glycols

Related event
29th European Symposium on Applied Thermodynamics
15th Annual Conference of the International Association for Mathematical Geosciences
Period: 2 Sep 2013
Thomas Mejer Hansen (Organizer)
Center for Energy Resources Engineering
National Space Institute
Mathematical and Computational Geoscience

Description
Session 20: Geostatistical priors in inversion of geophysical and engineering data
Conveners: Klaus Mosegaard (Technical University of Denmark, DENMARK), Thomas Mejer Hansen (Technical University of Denmark, DENMARK)
This session will explore current research in integration of geostatistical information with geophysical or engineering data. Special focus will be on new ideas and methods for incorporating geological realism into the solution of inverse problems such as history matching and seismic inversion.

Related event
15th Annual Conference of the International Association for Mathematical Geosciences: Frontiers of Mathematical Geosciences: New approaches to understand the natural World
02/09/2013 → 06/09/2013
Madrid, Spain
Activity: Attending an event › Participating in or organising a conference

BINARY VLE of DEEA/H2O, MAPA/H2O and DEEA/MAPA SYSTEMS
Period: 5 Jun 2013
Muhammad Waseem Arshad (Speaker)
Center for Energy Resources Engineering
Department of Chemical and Biochemical Engineering
CERE – Center for Energy Resources Engineering

Description
Oral Presentation by Ardi Hartono, Fahad Saleem, Muhammad Waseem Arshad, Muhammad Usmana and Hallvard F. Svendsen
Documents:
prod21371141562601.Ardi_Waseem_TCCS7_Final.pdf

Related event
7th Trondheim CCS Conference
04/06/2013 → 06/06/2013
Trondheim, Norway
Activity: Talks and presentations › Conference presentations

Design of a Tank Cleaning Blend through a Systematic Emulsified Product Design Methodology
Period: 20 Apr 2013 → 25 Apr 2013
Georgios Kontogeorgis (Lecturer)
Department of Chemical and Biochemical Engineering
Computer Aided Process Engineering Center
Center for Energy Resources Engineering
CERE – Center for Energy Resources Engineering

Description
Oral conference presentation: Michele Mattei, Peter Krogh, Bo Depner, Georgios M. Kontogeorgis and Rafiqul Gani, 2013, "Design of a Tank Cleaning Blend through a Systematic Emulsified Product Design Methodology"
**Related event**

**9th European Congress of Chemical Engineering**  
21/04/2013 → 25/04/2013  
The Hague, Netherlands  
Activity: Talks and presentations › Conference presentations

**Design of a Tank Cleaning Blend through a Systematic Emulsified Product Design Methodology**  
Period: 20 Apr 2013 → 25 Apr 2013  
Michele Mattei (Lecturer)  
Department of Chemical and Biochemical Engineering  
Computer Aided Process Engineering Center  
Center for Energy Resources Engineering  
CERE – Center for Energy Resources Engineering

**Description**  
Oral conference presentation: Michele Mattei, Peter Krogh, Bo Depner, Georgios M. Kontogeorgis and Rafiqul Gani, 2013, “Design of a Tank Cleaning Blend through a Systematic Emulsified Product Design Methodology”

**Related event**

**9th European Congress of Chemical Engineering**  
21/04/2013 → 25/04/2013  
The Hague, Netherlands  
Activity: Talks and presentations › Conference presentations

**Thermodynamic modeling of sour gas cleaning process with alkanolamines: Oral presentation at the 25th European Symposium on Applied Thermodynamics (ESAT), St.Petersburg, Russia**  
Period: 1 Jan 2011 → …  
Negar Sadegh (Speaker)  
Department of Chemical and Biochemical Engineering  
CERE – Center for Energy Resources Engineering

**Related event**

Thermodynamic modeling of sour gas cleaning process with alkanolamines: ESAT
Activity: Talks and presentations › Conference presentations

Thermodynamic modeling of sour gas cleaning process with alkanolamine: Oral presentation at the 25th European SYmposium on Applied Thermodynamics (ESAT), St.Petersburg, Russia
Period: 1 Jan 2011 → …
Georgios Kontogeorgis (Speaker)
Department of Chemical and Biochemical Engineering
CERE – Center for Energy Resources Engineering

Thermodynamic modeling of sour gas cleaning process with alkanolamine: Oral presentation at the 25th European SYmposium on Applied Thermodynamics (ESAT), St.Petersburg, Russia
Period: 1 Jan 2011 → …
Erling Halfdan Stenby (Speaker)
Department of Chemistry
Center for Energy Resources Engineering

Thermodynamic modeling of sour gas cleaning process with alkanolamine: Oral presentation at the 25th European SYmposium on Applied Thermodynamics (ESAT), St.Petersburg, Russia
Period: 1 Jan 2011 → …
Kaj Thomsen (Speaker)
Department of Chemical and Biochemical Engineering
CERE – Center for Energy Resources Engineering

Thermodynamic modeling of sour gas cleaning process with alkanolamine: Presented at (oral presentation) CERE discussion meeting, Hillerød
Period: 1 Jan 2011 → …
Negar Sadegh (Speaker)
Department of Chemical and Biochemical Engineering
CERE – Center for Energy Resources Engineering

Related external organisation
Unknown external organisation
Activity: Talks and presentations › Conference presentations

Related external organisation
Unknown external organisation
Activity: Talks and presentations › Conference presentations

Related external organisation
Unknown external organisation
Activity: Talks and presentations › Conference presentations
Thermodynamic modeling of sour gas cleaning process with alkanolamine: Presented at (oral presentation) CERE discussion meeting, Hillerød
Period: 1 Jan 2011 → …
Georgios Kontogeorgis (Speaker)
Department of Chemical and Biochemical Engineering
CERE – Center for Energy Resources Engineering

Related external organisation
Unknown external organisation
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Thermodynamic modeling of sour gas cleaning process with alkanolamine: Presented at (oral presentation) CERE discussion meeting, Hillerød
Period: 1 Jan 2011 → …
Erling Halfdan Stenby (Speaker)
Department of Chemistry
Center for Energy Resources Engineering

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Kaj Thomsen (Speaker)
Department of Chemical and Biochemical Engineering
CERE – Center for Energy Resources Engineering
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Unknown external organisation
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