Center for Energy Resource Engineering (CERE) is a continuation of Center for Phase Equilibria and Separation Processes (IVC-SEP). CERE's main activities lie within applied thermodynamics, interface- and colloidal chemistry, geology and scientific computing. The center combines a range of disciplines of great importance in oil and gas production, CO2 capture and storage (CCS) and geothermal power. Additionally, the center carries out generic research within the fundamental disciplines.

Research results are applied to processes and products in the industry with a main focus on energy, environment and advanced materials. A substantial part of the center's research has been dedicated to Enhanced Oil Recovery (EOR). Head of CERE per 1.7.2014 is professor Georgios M. Kontogeorgis.

Publications:

CO2 Mass transfer model for carbonic anhydrase-enhanced aqueous MDEA solutions

In this study a CO2 mass transfer model was developed for carbonic anhydrase-enhanced MDEA solutions based on a mechanistic kinetic enzyme model. Four different enzyme models were compared in their ability to predict the liquid side mass transfer coefficient at temperatures in the range of 298 to 328 K, solvent concentrations in the range 15 to 50 wt%, CO2 partial pressures up to 50 kPa, solvent loading between 0 and 0.5 mole CO2 per mole MDEA and enzyme concentrations up to 8.5 g/L. The reversible Michaelis Menten model (MR) and the simplified model with product inhibition by the bicarbonate ion (SP) were able to predict the mass transfer with an absolute average relative deviation of less than 15%. The MR model could account for every influence (solvent concentration, temperature, solvent loading, CO2 partial pressure) of the different process conditions on the mass transfer, whereas the SP model is limited to applications with low CO2 partial pressure such as CCS from coal burning power plants. Two other models that were also investigated are not suitable for implementation into an absorber column simulation, as they cannot describe the influence of changing solvent loading on the mass transfer.
Estimation of Physical Properties of Amino Acids by Group-Contribution Method

In this paper, we present group-contribution (GC) based property models for estimation of physical properties of amino acids using their molecular structural information. The physical properties modelled in this work are normal melting point ($T_{\text{m}}$), aqueous solubility ($W_{\text{a}}$), and octanol/water partition coefficient ($K_{\text{ow}}$) of amino acids. The developed GC-models are based on the published GC-method by Marrero and Gani (J. Marrero, R. Gani, Fluid Phase Equilib. 2001, 183-184, 183-208) with inclusion of new structural parameters (groups and molecular weight of compounds). The main objective of introducing these new structural parameters in the GC-model is to provide additional structural information for amino acids having large and complex structures and thereby improve predictions of physical properties of amino acids. The group-contribution values were calculated by regression analysis using a data-set of 239 values for $T_{\text{m}}$, 211 values for $W_{\text{a}}$, and 335 values for $K_{\text{ow}}$. Compared to other currently used GC-models, the developed models make significant improvements
in accuracy with average absolute error of 10.8 K for Tm and logarithm-unit average absolute errors of 0.16 for K_{ow} and 0.19 for W_{s}.

**General information**

State: Published
Organisations: Department of Chemical and Biochemical Engineering, KT Consortium, CERE – Center for Energy Resources Engineering, Alfa Laval
Authors: Jhamb, S. V. (Intern), Liang, X. (Intern), Gani, R. (Intern), Hukkerikar, A. S. (Ekstern)
Pages: 148-161
Publication date: 2018
Main Research Area: Technical/natural sciences

**Publication information**

Journal: Chemical Engineering Science
Volume: 175
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Ratings:
- BFI (2018): BFI-level 2
- BFI (2017): BFI-level 2
- 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
- BFI (2009): BFI-level 2
- 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
Hydrate thermal dissociation behavior and dissociation enthalpies in methane-carbon dioxide swapping process

The swapping of methane with carbon dioxide in hydrate has been proposed as a potential strategy for geologic sequestration of carbon dioxide and production of methane from natural hydrate deposits. However, this strategy requires a better understanding of the thermodynamic characteristics of CH₄ and CO₂ hydrate as well as (CH₄ + CO₂) or (CH₄ + CO₂ + N₂) mixed hydrates (since (CO₂ + N₂) gas mixture is often used as the swapping gas), along with the thermal physics property changes during gas exchange. In this study, a high pressure micro-differential scanning calorimetry (HP μ-DSC) was performed on synthesized gas hydrates to investigate the dissociation behavior of various hydrates. The hydrate dissociation enthalpies were determined by both μ-DSC measurement and Clapeyron equation. For the single guest molecule hydrate system, the average dissociation enthalpies of CH₄ hydrate and CO₂ hydrate measured by integrating the endothermic peak area are 55.01 kJ·mol⁻¹ and 58.96 kJ·mol⁻¹, respectively, which are very close to the values calculated by Clapeyron equation. However, in the multicomponent guest hydrates system, the μ-DSC measured dissociation enthalpies of the (CH₄ + CO₂) binary hydrates and (CH₄ + CO₂ + N₂) ternary hydrates are a little higher than that of Clapeyron equation, it was found that their dissociation enthalpies are located between the limiting values of pure CH₄ hydrate and CO₂ hydrate, increasing with the mole fraction of CO₂ in hydrate phase. By monitoring the heat flow changes with the μ-DSC apparatus, it was observed that there was no noticeable dissociation or reformation process of hydrate occurring in the CH₄ − CO₂/(CO₂ + N₂) swapping, which indicates that most CH₄ hydrate forms (CH₄ + CO₂) or (CH₄ + CO₂ + N₂) mixed hydrates directly instead of dissociating into liquid water or ice first. The dissociation equilibrium data obtained from the endothermic thermograms of the mixed hydrates after CO₂ and (CO₂ + N₂) swapping demonstrates that about 66% and 85% of CH₄ in hydrate phase are replaced, respectively.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering
Authors: Mu, L. (Intern), von Solms, N. (Intern)
Pages: 33-42
Publication date: 2018
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Chemical Thermodynamics
Volume: 117
ISSN (Print): 0021-9614
Ratings:
BFI (2018): BFI-level 2
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
BFI (2014): BFI-level 1
Near-wellbore modeling of a horizontal well with Computational Fluid Dynamics

The oil production by horizontal wells is a complex phenomenon that involves flow through the porous reservoir, completion interface and the well itself. Conventional reservoir simulators can hardly resolve the flow through the completion into the wellbore. On the contrary, Computational Fluid Dynamics (CFD) is capable of modeling the complex interaction between the creeping reservoir flow and turbulent well flow for single phases, while capturing both the completion geometry and formation damage. A series of single phase steady-state simulations are undertaken, using such fully coupled three dimensional numerical models, to predict the inflow to the well. The present study considers the applicability of CFD for near-wellbore modeling through benchmark cases with available analytical solutions. Moreover, single phase steady-state numerical investigations are performed on a specific perforated horizontal well producing from the Siri field, offshore Denmark. The performance of the well is investigated with an emphasis on the inflow profile and the productivity index for different formation damage scenarios. A considerable redistribution of the inflow profile were found when the filtrate invasion extended beyond the tip of the perforations.

General information
State: Published
New association schemes for mono-ethylene glycol: Cubic-Plus-Association parameterization and uncertainty analysis

Accurate thermodynamic predictions for systems containing glycols are essential for the design and commissioning of novel subsea natural gas dehydration units. Previously it has been shown that the Cubic-Plus-Association (CPA) equation of state can be used to model VLE, SLE and LLE for mixtures of interest to this application. Recent developments for association schemes have shown that the use of a binary association site provided improved modelling of 1-alkanols. In this work, we implement the binary association site for mono-ethylene glycol (MEG) by proposing three new association schemes (3C, 4E & 4F). New parameter sets have been regressed and uncertainty analysis, using the bootstrap methodology, was performed to obtain 95% confidence intervals for each parameter. An improved parameter set for the literature 4C scheme was also determined.

The four association schemes were tested against eight data types, with single parameter sensitivity analysis showing that new parameter sets are near optimal. The 3C scheme provides the best results for pure component properties and the liquid phase of MEG-H₂O, while new 4C parameters provide the best results for the MEG-H₂O (vapour phase) and MEG-nC₇ LLE. For the limited ternary (MEG-H₂O-CH₄) data and MEG-nC₆ LLE, the best results are achieved using the 4F scheme. Ternary modelling performance was further improved by using binary interaction parameters fitted to binary vapour phase data.

While each of the new parameter sets provided an improvement over the literature parameters, it was found that no specific scheme was universally the best option. Given the uncertainty ranges and inconsistency between literature data, additional experimental data are required.

Despite the lack of sufficient data, the value of the bootstrap method has been highlighted, both for finding improved parameter sets and transferring uncertainty from experimental data through to thermodynamic and process models.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CERE – Center for Energy Ressources Engineering, KT Consortium
Authors: Kruger, F. (Intern), Kontogeorgis, G. M. (Intern), von Solms, N. (Intern)
Pages: 211–233
Publication date: 2018
Main Research Area: Technical/natural sciences

Publication information
Journal: Fluid Phase Equilibria
Volume: 458
ISSN (Print): 0378-3812
Ratings:
BFI (2018): BFI-level 2
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
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 Ressources Engineering, Department of Chemistry, Asphalteam
Application of a Crossover Equation of State to Describe Phase Equilibrium and Critical Properties of n-Alkanes and Methane/n-Alkane Mixtures

Crossover equations of state (EOSs) are models that incorporate density fluctuations into mean-field thermodynamic models, changing their behavior close to the critical point. In this way, they are capable of describing the analytical behavior of fluids far from the critical region and the asymptotic one near the critical point. Although several crossover EOSs have been developed in the last decades their use in modeling industrial processes is rather limited. In this work, we use the crossover Soave–Redlich–Kwong (CSRK) to describe phase equilibrium and critical properties of pure n-alkanes and methane/n-alkane binary mixtures and compare the results to two other modeling approaches of the SRK EOS. In the case of the pure fluids, CSRK gives an accurate overall description of the phase equilibrium and critical properties; nevertheless, a minor increase in the deviation of the saturation pressure and other properties is observed when compared to that of the mean-field model. For the binary mixtures, an improvement in the description of the critical volumes is seen, while, for the other properties, similar results are obtained.

General information
State: Accepted/In press
Organisations: Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering, Department of Chemistry, KT Consortium
Authors: P. C. M. Vinhal, A. (Intern), Yan, W. (Intern), Kontogeorgis, G. M. (Intern)
Number of pages: 13
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Chemical and Engineering Data
ISSN (Print): 0021-9568
Ratings:
BFI (2018): BFI-level 2
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
Calculation of Multiphase Chemical Equilibrium by the Modified RAND Method

A robust and efficient algorithm for simultaneous chemical and phase equilibrium calculations is proposed. It combines two individual nonstoichiometric solving procedures: a nested-loop method with successive substitution for the first steps and final convergence with the second-order modified RAND method. The modified RAND extends the classical RAND method from single-phase chemical reaction equilibrium of ideal systems to multiphase chemical equilibrium of nonideal systems. All components in all phases are treated in the same manner and the system Gibbs energy can be used to monitor convergence. This is the first time that modified RAND was applied to multiphase chemical equilibrium systems. The combined algorithm was tested using nine examples covering vapor–liquid (VLE) and vapor–liquid–liquid equilibria (VLLE) of ideal and nonideal reaction systems. Successive substitution provided good initial estimates for the accelerated computation with modified RAND, to ultimately converge to the equilibrium solution without failure.

General information
State: Published
Organisations: Department of Chemistry, CERE – Center for Energy Ressources Engineering, Technical University of Denmark
Authors: Tsanas, C. (Ekstern), Stenby, E. H. (Intern), Yan, W. (Intern)
Pages: 11983-11995
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Industrial and Engineering Chemistry Research
Volume: 56
Issue number: 41
ISSN (Print): 0888-5885
Ratings:
BFI (2018): BFI-level 2
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
CO2 Capture with Liquid-Liquid Phase Change Solvents: A Thermodynamic Study

Extended UNIQUAC thermodynamic framework was implemented in this work to model the aqueous blend of N, N-Diethylethanolamine (DEEA) and N-Methyl-1,3-diaminopropane (MAPA) for CO2 capture. The model parameters were estimated first for the two ternary systems, H2O-DEEA-CO2 and H2O-MAPA-CO2, followed by the quaternary H2O-DEEAMAPA-CO2 system which gives liquid-liquid phase split when reacted with carbon dioxide. A total of 94 model parameters and 6 thermodynamic properties were fitted to approximately 1500 equilibrium and thermal experimental data consisting of pureamine vapor pressure (Pvap), vapor-liquid equilibrium (VLE), solid-liquid equilibrium (SLE), liquid-liquid equilibrium (LLE), excess enthalpy (HE), and heat of absorption (ΔHabs) of CO2 in aqueous amine solutions. The model
developed in this work can accurately represent the equilibrium and thermal data for the studied systems with a single unique set of parameters.

**General information**

State: Published

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


Pages: 1671 – 1681

Publication date: 2017


Main Research Area: Technical/natural sciences

**Publication information**

Journal: Energy Procedia

Volume: 114

ISSN (Print): 1876-6102

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BFI (2018): BFI-level 1

BFI (2017): BFI-level 1

BFI (2016): BFI-level 1

Scopus rating (2016): CiteScore 1.16 SJR 0.467 SNIP 0.586

Web of Science (2016): Indexed yes

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

Scopus rating (2010): SJR 0.433 SNIP 0.957

Web of Science (2009): Indexed yes

Original language: English

Thermodynamic modeling, Extended UNIQUAC, Phase change solvents, DEEA, MAPA, Liquid-liquid equilibrium, CO2 capture

Electronic versions:

CO2_Capture_with_Liquid_Liquid_Phase_Change_Solvents.pdf

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Publication: Research - peer-review » Conference article – Annual report year: 2016

**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 Vapour-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.
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 16,099bp 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, Department of Biotechnology and Biomedicine, Center for Energy Resources Engineering, Department of Chemical and Biochemical 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)
Pages: 139-140
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Mitochondrial DNA Part B
Volume: 2
Issue number: 1
ISSN (Print): 2380-2359
Ratings:
Web of Science (2017): Indexed yes
Original language: English
Oriental hornet, Vespa orientalis F, Mitochondrial genome
Electronic versions:
Complete mitochondrial genome of the Oriental Hornet_Vespa orientalis F_Hymenoptera_Vespidae.pdf
DOI:
10.1080/23802359.2017.1292480

Bibliographical note
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Source: PublicationPreSubmission
Source-ID: 131183132
Considerations for implementation of novel enzyme-based processes

Biocatalysis is the use of enzymes to catalyze chemical reactions. It is an established synthesis route in chemical synthesis, alongside conventional chemistry. Biocatalysis is often applied due to excellent regio and stereoselectivity, in addition to its environmentally benign properties. This thesis aims at increasing the potential use of industrial biocatalysis, both in terms of broadening its current use and expanding it to new applications. This academic study is carried out through two case studies. These two case studies were chosen because they represent each end of the spectra of biocatalytic applications. The first case study is expanding the use of an established biocatalyst. The second case study investigates the potential of a novel biocatalyst. In addition, the two case studies have very different implementation challenges, impeding current use. Therefore, arguably, the lessons learned from these two case studies justify general conclusions for biocatalysis, irrespective of their application. The work in this thesis therefore contributes, not only to industrial biocatalysis in these two areas, but also increases the understanding of biocatalysis as a whole.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, PROSYS - Process and Systems Engineering Centre, KT Consortium, CERE – Center for Energy Resources Engineering
Authors: Deslauriers, M. G. (Intern), Woodley, J. (Intern), von Solms, N. (Intern)
Number of pages: 203
Publication date: 2017

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)
Pages: 2592-2605
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Chemical and Engineering Data
Volume: 62
Issue number: 9
ISSN (Print): 0021-9568
Ratings:
BFI (2018): BFI-level 2
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
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 0.661 SNIP 1.062
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 0.978 SNIP 1.234
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 0.735 SNIP 1.16
Design and simulation of rate-based CO₂ capture processes using carbonic anhydrase (CA) applied to biogas

Today the mix of the energy sector is changing from reduction of CO₂ emission from fossil fueled power industry into a general focus on renewable industry which is emitting less greenhouse gases. Renewable fuels like biomass for electricity production or biogas for bio-methane production have a potential to create negative emissions using bio-energy carbon capture and storage (BECCS).

All sectors are still in the need for applying more sustainable carbon capture and storage (CCS) technologies which result in lower energy consumption while reducing the impact on the environment. Recently several promoters have been developed for solvent based technologies, but there is still a need to develop new approaches which can potentially reduce energy consumption even further. Solvents typically used for CCS have the tendency to form carbamate. They are characterized by the speed at which they react with CO₂. Advantageous kinetics results in smaller equipment size. But this is not the only benefit.

In this study we deliberately apply a slow reacting solvent, MDEA (methyl-diethanolamine). It is in the category of noncarbamate forming tertiary amines, for the same reason it binds less hard to CO₂. The advantage is a noticeably lower regeneration energy compared to primary and secondary amines. As a result the cost for stripping is significantly lower. Reactivated slow tertiary amines are applied in this study with the aim of reducing energy consumption. This is achieved by using carbonic anhydrase (CA) enzymes as additives in the slow solvent. The aim of this work is to develop a rate-based model for tertiary MDEA mixed with various amounts of CA. The results show that the properties for biogas are significantly different compared to air and may need to be treated accordingly accurate. This work proves that the typical mass transfer resistance observed in the biogas gas phase is low compared to the resistance in the liquid phase. The consequence is a reduced requirement for accurate properties for the biogas and the biogas can easily be modelled as being similar to air. In this work we create a calculation engine which is capable of BECCS, thereby enabling prevention of CO₂ emissions from renewable technologies giving a potential for zero-emission scenarios which can help to reach the new low emission CO₂ target set up by COP21
Design, economics and parameter uncertainty in dynamic operation of post-combustion CO₂ capture using piperazine (PZ) and MEA

Post-combustion capture is a promising solution to mitigate the anthropogenic CO₂ emission rate and reduce global warming. However, to make it economically attractive, the techno-economic performance of this process needs to be improved. This includes steady-state but also dynamic operation of the plant. Flexibility is particularly crucial from an economic and operational point of view since plants must balance the power production and the electricity demand on a daily basis.

This work shows the impact of design decisions and uncertainties on the dynamic operation and economics of a CO₂ capture plant using piperazine (PZ), compared to the benchmark MEA solvent. This is exemplified through dynamic model calculations. The results show that the capacity of the buffer tank is a key parameter for the flexibility of the plant. A small tank corresponds to lower capital cost but it leads to increased operation cost and also to flexibility/controllability issues. Both, the PZ and MEA plants present inverse response for small tanks. These plants are challenging to control.

General information
State: Published
Organisations: Department of Applied Mathematics and Computer Science, Scientific Computing, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering, University of Waterloo
Authors: Gaspar, J. (Intern), Ricardez-Sandoval, L. (Ekstern), Jørgensen, J. B. (Intern), Fosbøl, P. L. (Intern)
Pages: 1444-1452
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Journal: Energy Procedia
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Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.16 SJR 0.467 SNIP 0.586
Web of Science (2016): Indexed yes
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
Determination of Zinc Sulfide Solubility to High Temperatures

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.
Dimerization of Carboxylic Acids: An Equation of State Approach

The association term of the nonrandom hydrogen bonding theory, which is an equation of state model, is extended to describe the dimerization of carboxylic acids in binary mixtures with inert solvents and in systems of two different acids. Subsequently, the model is applied to describe the excess enthalpies and the vapor-liquid equilibrium of relevant binary mixtures containing low molecular weight organic acids. The model sheds light on the interplay of intermolecular interactions through the calculation of the various contributions to the mixing enthalpies, namely from hydrogen bonding and non-hydrogen bonding (dipolar, induced polar or dispersive) interactions. According to model predictions, the acid molecules are so strongly associated that the addition of inert solvents to carboxylic acids with small carbon numbers at ambient temperature does not dramatically alter their degree of association. Consequently, the observed endothermic dissolution process is mainly attributed to the hindering of polar interactions. Furthermore, upon mixing of two carboxylic acids, the rearrangement of hydrogen bonds due to the formation of cross associating species results in an insignificant contribution to the heats of mixing due to the rather constant dimerization enthalpy that is revealed by the available experimental data for low molecular weight compounds.

General information
State: Published
Organisations: CERE – Center for Energy Ressources Engineering, Department of Chemical and Biochemical Engineering, Aristotle University of Thessaloniki
Authors: Tsivintzelis, I. (Ekstern), Kontogeorgis, G. (Intern), Panayiotou, C. (Ekstern)
Pages: 2153-2163
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Publication information
Journal: Journal of Physical Chemistry Part B: Condensed Matter, Materials, Surfaces, Interfaces & Biophysical
Volume: 121
Issue number: 9
ISSN (Print): 1520-6106
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.03 SJR 1.348 SNIP 1.02
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
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Journal: Fluid Phase Equilibria
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BFI (2018): BFI-level 2
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
Elasticity and electrical resistivity of chalk and greensand during water flooding with selective ions

Water flooding with selective ions has in some cases lead to increased oil recovery. We investigate the physical processes on a pore scale that are responsible for changes in petrophysical and mechanical properties of four oil-bearing chalk and four oil-bearing greensand samples caused by flooding with brines containing varying amounts of dissolved NaCl, Na₂SO₄, MgCl₂ and MgSO₄. Ultrasonic P-wave velocity and AC resistivity measurements were performed prior to, during and after flow through experiments in order to identify and quantify the processes related to water flooding with selective ions. Low field Nuclear Magnetic Resonance (NMR) spectrometry measurements were performed at full water saturation, at irreducible water saturation, after aging and after flooding. Low field NMR data indicates changes in the pore fluid distribution and wettability of chalk after aging of one of the samples. NMR data for other samples indicate that chalk is water-wet after flooding. Greensand remained mixed wet throughout the experiments. Electrical resistivity data are in agreement with this interpretation. The electrical resistivity data during flooding revealed that the formation brine is not fully replaced by the injected water in both chalk and greensand. Changes in the elasticity of chalk during flooding illustrate the softening effect of magnesium bearing brines as compared to the sodium bearing brines. The stiffness of greensand was not affected by water flooding with selective ions as determined from the elastic wave measurements. Precipitation of fines during flooding of chalk samples is indicated by an increase in specific surface area and a shift in the MICP to lower values but no fines were detected by NMR. No changes were observed for greensand samples.

General information
State: Accepted/In press
Organisations: Department of Civil Engineering, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Ressources Engineering, Department of Chemistry, Section for Geotechnics and Geology, University Savoie Mont Blanc, Politecnico di Torino
Number of pages: 54
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Main Research Area: Technical/natural sciences

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Journal: Journal of Petroleum Science and Engineering
ISSN (Print): 0920-4105
Ratings:
BFI (2018): BFI-level 1
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
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Main Research Area: Technical/natural sciences

Publication information
Journal: Langmuir
Volume: 33
Issue number: 18
ISSN (Print): 0743-7463
Ratings:
BFI (2018): BFI-level 1
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
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 2.051 SNIP 1.357 CiteScore 4.42
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 2.148 SNIP 1.4
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 2.156 SNIP 1.351
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 2.383 SNIP 1.34
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 2.449 SNIP 1.434
Web of Science (2007): Indexed yes
Evaluation of equations of state for simultaneous representation of phase equilibrium and critical phenomena

Precise description of the critical points with association equations of state requires rescaling of the parameters to match experimental critical temperature and pressure of pure components. In this work we developed a method to include critical data restrictions in the parametrization procedure of the Cubic-Plus-Association (CPA) equation of state (EoS). We obtained new parameters for methanol and alkanes from n-hexane to n-decane. The comparison with the original parameters showed that this procedure is important for associating compounds, since for inert species the equation reduces to the Soave-Redlich-Kwong (SRK) EoS. The application of the rescaled parameters improved the critical point representation of pure fluids at the expense of the saturated liquid phase volume description. In the case of binary mixtures containing methanol and n-alkanes, the association model with the new parameters satisfactorily predicted the experimental critical data, indicating the importance of the rescaling parametrization procedure in the computation of the critical pressure and temperature for systems with associating species. Both sets of CPA parameters gave similar deviations in the bubble point pressure and vapor composition for the vapor-liquid equilibrium calculations. However, the rescaled parameters gave rise to larger deviations in the composition of the polar rich phase in the liquid-liquid equilibrium.
Extension of modified RAND to multiphase flash specifications based on state functions other than (T,P)

The recently proposed modified RAND formulation is extended from isothermal multiphase flash to several other state function based flash specifications. The obtained general formulation is applicable to chemical equilibrium although this study is focused on flash with only phase equilibrium. It is demonstrated that a common symmetric Jacobian matrix can be formulated for all of these flash specifications. Newton iteration with the common Jacobian is used to converge for the majority of cases and a Q-function maximisation with nested isothermal flash in the inner loop is used for the non-convergent exceptions. For isothermal flash with modified RAND, it can happen in rare occasions that the modified RAND
step is ascending in the Gibbs energy. A correction of the step is proposed for such cases to obtain a descent direction without violating the condition used in the derivation of modified RAND. A two-phase example is used to demonstrate that the described method is suitable for (H,P), (T,V), (S,V) and (U,V) flash specifications and a four-phase case is examined in more detail for the difficult (U,V) case. Two- and three-phase examples close to critical regions are used to demonstrate the effectiveness of the correction procedure for the modified RAND step and to show that satisfactory rates of convergence are obtained.

General information
State: Published
Organisations: Department of Chemistry, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Ressources Engineering
Authors: Paterson, D. (Intern), Michelsen, M. L. (Intern), Yan, W. (Intern), Stenby, E. H. (Intern)
Pages: 288-299
Publication date: 2017
Main Research Area: Technical/natural sciences

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Journal: Fluid Phase Equilibria
Volume: 458
ISSN (Print): 0378-3812
Ratings:
BFI (2018): BFI-level 2
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
First Study of Poly(3-Methylene-2-Pyrrolidone) as a Kinetic Hydrate Inhibitor

Formation of gas hydrates is a problem in the petroleum industry where the gas hydrates can cause blockage of the flowlines. Kinetic hydrate inhibitors (KHIs) are water-soluble polymers, sometimes used in combination synergistically or with non-polymeric synergists, that are used to prevent gas hydrate blockages. They have been used in the field successfully since 1995. In this paper, we present the first KHI results for the polymer, poly(3-methylene-2-pyrrolidone) (P(3M2P)), which is structurally similar to poly(N-vinylpyrrolidone) (PVP), one of the first KHIs to be discovered. 3M2P polymers with different molecular weights (5500 and 2500 g/mole) and at different concentrations (2500, 5000 and 7500 ppm) were investigated for their KHI performance on SII hydrates in high-pressure rocking cells. We also investigated the synergistic effect of P(3M2P) with n-butyl glycol ether (BGE), a known synergist for some KHI polymers. At the lower concentrations, P(3M2P) gives a similar performance to PVP (Mw = 8000-9000 g/mole). However, PVP outperforms both samples of P(3M2P) at 7500 ppm, with and without BGE. We suggest that the reasons for the performance level of P(3M2P) are related to greater resonance stabilization of the amide group in P(3M2P) compared to PVP. Also, the pyrrolidone ring of the PVP repeat unit has a larger hydrophobic sequence of three methylene units compared to the two methylene units in the pyrrolidone ring of P(3M2P). This relates well to previous studies where larger hydrophobic groups are preferable in KHI polymers as long as they are water-soluble at hydrate-forming temperatures.
Freezing Point Determination of Water–Ionic Liquid Mixtures
Freezing points of aqueous solutions of HOEtPyBr, HOEtMimBr, AmimCl, EtOMimCl, EmimDep, and EmimAc were measured using a modified Beckmann apparatus with automatic data logging. The ionic liquids (ILs) in this study exhibited features similar to those of inorganic salts in depressing the freezing point of water. On the basis of the cryoscopic behavior recorded, the solid phases formed at higher IL contents were presumed to be hydrates of the form IL·nH2O. The HOEtPyBr·H2O and HOEtMimBr·H2O systems formed simple eutectic systems. The eutectic points were found to be at a water mole fraction of 0.617 and 219.841 K in the first system and at a water mole fraction of 0.657 and 202.565 K in the second system. Water activities in aqueous IL solutions were predicted by COSMO-RS and COSMO-SAC and compared to water activities derived from the experimentally determined freezing points. The COSMO-RS predictions were closer to the experimental water activities than the COSMO-SAC predictions. The experimental results indicate that the freezing points of IL+H2O systems are affected by the nature of both cations and anions. However, according to the COSMO-RS excess enthalpy predictions, the anions have a relatively higher influence than cations on the IL+H2O interaction.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering, CERE – Center for Energy Resources Engineering, Chinese Academy of Sciences
Authors: Liu, Y. (Intern), Meyer, A. S. (Intern), Nie, Y. (Ekstern), Zhang, S. (Ekstern), Zhao, Y. (Ekstern), Fosbøl, P. L. (Intern), Thomsen, K. (Intern)
Pages: 2374–2383
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
General approach for solving the density gradient theory in the interfacial tension calculations

Within the framework of the density gradient theory, the interfacial tension can be calculated by finding the density profiles that minimize an integral of two terms over the system of infinite width. It is found that the two integrands exhibit a constant difference along the interface for a finite planar interface, and this difference becomes smaller as the interface width increases. These findings naturally lead to a solution procedure that consists of an inner loop and an outer loop for calculating the interfacial tension of a planar interface. The outer loop deals with the relationship between the interfacial tension and the interface width, and it permits us to obtain accurate results from finite width calculations. The inner loop minimizes the interfacial tension for a given interface width by adjusting the density profiles, in which the integrals are evaluated by a combination of Gauss-Lobatto quadrature and Lagrange interpolation based polynomial approximation. A better approximation of the interfacial tension is derived by a path integration along the density profiles. These strategies enable us to obtain accurate solutions with looser tolerance criteria and a fewer number of thermodynamic property evaluations compared to other methods. The performance of the algorithm with recommended parameters is analyzed for various systems, and the efficiency is further compared with the geometric-mean density gradient theory, which only needs to solve nonlinear algebraic equations. The results show that the algorithm is only 5-10 times less efficient than solving the geometric-mean density gradient theory.

General information
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Organisations: Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering, KT Consortium
Authors: Liang, X. (Intern), Michelsen, M. L. (Intern)
Pages: 79-90
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Main Research Area: Technical/natural sciences

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Volume: 451
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Ratings:
BFI (2018): BFI-level 2
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
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.
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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.
Improvement of predictive tools for vapor-liquid equilibrium based on group contribution methods applied to lipid technology

Predictive methodologies based on group contribution methods, such as UNIFAC, play a very important role in the design, analysis and optimization of separation processes found in oils, fats and biodiesel industries. However, the UNIFAC model has well-known limitations for complex molecular structures that the first-order functional groups are unable to handle. In the particular case of fatty systems these models are not able to adequately predict the non-ideality in the liquid phase. Consequently, a new set of functional groups is proposed to represent the lipid compounds, requiring thereby, new group interaction parameters. In this work, the performance of several UNIFAC variants, the Original-UNIFAC, the Linear-UNIFAC, Modified-UNIFAC and the Dortmund-UNIFAC is compared. The same set of experimental data and the parameter estimation method developed by Perederic et al. (2017) have been used. The database of measured data comes from a special lipids database developed in-house (SPEED Lipids database at KT-consortium, DTU, Denmark). All UNIFAC models using the new lipid-based parameters show, on average, improvements compared to the same models with their published parameters. There are rather small differences between the models and no single model is the best in all cases.

General information
State: Accepted/In press
Organisations: Department of Chemical and Biochemical Engineering, KT Consortium, CERE – Center for Energy Resources Engineering, Technical University of Denmark, University of Campinas
Authors: Damaceno, D. S. (Ekstern), Perederic, O. A. (Intern), Ceriani, R. (Ekstern), Kontogeorgis, G. M. (Intern), Gani, R. (Intern)
Influence of temperature and solvent concentration on the kinetics of the enzyme carbonic anhydrase in carbon capture technology

In this study the effect of carbonic anhydrase addition on the absorption of CO$_2$ was investigated in a wetted wall column apparatus. Four different solvents: the primary amine monoethanolamine (MEA), the sterically hindered primary amine 2-amino-2-methyl-1-propanol (AMP), the tertiary amine N-methyl-diethanolamine (MDEA) and the carbonate salt solution K$_2$CO$_3$ were compared in concentrations from 5 to 50 wt% in a temperature range of 298–328 K with and without enzyme. Necessary mass transfer parameters such as liquid side mass transfer coefficient and solvent and enzyme reaction rates were determined and benchmarked to a 30 wt% MEA solution. The study reveals that the addition of the enzyme carbonic anhydrase (CA) dramatically increases the liquid side mass transfer coefficient for MDEA, and K$_2$CO$_3$; AMP has a moderate increase whereas MEA was unchanged. The results confirm that just bicarbonate forming systems benefit from CA. The influence of temperature on the enzyme kinetics and mass transfer coefficients is different for different solvent types. A temperature increase resulted in lower liquid side mass transfer coefficient for MDEA and K$_2$CO$_3$ but in a higher coefficient for AMP. The overall first order enzyme reaction rate (s$^{-1}$) was linearly dependent on enzyme concentration for MDEA and K$_2$CO$_3$ at 313 K. Temperature and concentration did increase the enzymatic rate constant slightly in the concentration range of 5–15 wt% K$_2$CO$_3$ and significantly between 15 and 20 wt%. The enzymatic reaction rate constant for MDEA decreased with temperature, the solvent concentration had a negligible on it. The enzymatic reaction rate for AMP rose with temperature and was higher for lower solvent concentration.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CERE – Center for Energy Ressources Engineering, CAPEC-PROCESS
Authors: Gladis, A. (Intern), Deslauriers, M. G. (Intern), Fosbøl, P. L. (Intern), Woodley, J. (Intern), von Solms, N. (Intern)
Pages: 772-786
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Biochemical Engineering Journal
Volume: 309
ISSN (Print): 1369-703x
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.16
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 2.75
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 2.72
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 3.03
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1

The book Classical Thermodynamics of Fluid Systems: Principles and Applications written by professor Juan H. Vera and Dr. Grazyna Wilczek-Vera is undoubtedly a book written in a most personal style by the two distinguished authors. The book contains four sections and a fifth one with appendices (mostly on selected thermodynamic models). The first two sections contain a total of 18 chapters on fundamentals of thermodynamics and mixtures, including phase diagrams. These chapters on the fundamentals are presented in a very rigorous, mathematical, and rather condensed way, in carefully formulated short chapters, with a minimum number of figures, tables, examples, and references. The terminology and nomenclature is clear and consistent across the whole book. The interrelations between the thermodynamic properties and variables are presented in an exceptionally clear way and an excellent illustration of this is the equation on the cover page of Section II. Especially Chapters 14 and 15 present these interrelations of thermodynamic properties in a very comprehensive way. With the exception of Chapter 18 on electrolyte solutions, essentially no models which, as the authors say “come and go”, are presented in these first two sections. Electrolytes is an area of active research for many including the authors of the book and it is, thus, not surprising that extra attention to electrolytes is given in various places in the book, already in Section II. In addition to an entire chapter about electrolytes (Chapter 18), equilibrium involving ions is discussed in Chapter 10 and the use of molality as a measure of concentration in Chapter 15.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering, KT Consortium
Authors: Kontogeorgis, G. (Intern)
Pages: 1415-1416
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Continuum Mechanics and Thermodynamics
Volume: 29
Issue number: 6
ISSN (Print): 1432-0959
Ratings:
Scopus rating (2016): CiteScore 2.51 SNIP 1.394 SJR 1.418
Scopus rating (2015): CiteScore 1.43 SNIP 1.023 SJR 0.66
Scopus rating (2014): CiteScore 1.85 SNIP 1.36 SJR 0.911
Kinetic study of a Layout for the Carbon Capture with Aqueous Ammonia without Salt Precipitation

This paper focuses on carbon capture in an Ultra Super Critical power plant. The technology selected for CO\(_2\) capture is based on cooled ammonia scrubbing in post-combustion mode, as recently investigated by the authors in another work. Here, a rate-based approach is adopted. In detail, a specific primary energy consumption for CO\(_2\) avoided (SPECCA) of 2.77 MJ/kgCO\(_2\) is calculated in case of 85% of CO\(_2\) capture, with an ultimate power plant efficiency of 37.27%.

**General information**

State: Published
Organisations: Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering, Politecnico di Milano
Authors: Bonalumi, D. (Ekstern), Lillia, S. (Ekstern), Valenti, G. (Ekstern), Fosbøl, P. L. (Intern), Thomsen, K. (Intern)
Pages: 1352 – 1359
Publication date: 2017
Main Research Area: Technical/natural sciences

**Publication information**
Journal: Energy Procedia
Volume: 114
ISSN (Print): 1876-6102
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.16 SJR 0.467 SNIP 0.586
Web of Science (2016): Indexed yes
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
Methane Production and Carbon Capture by Hydrate Swapping

There are essentially two different approaches to producing methane from natural gas hydrate reservoirs, either bring the hydrate out of its thermodynamic stability region or expose the hydrate to a substance that will form a more stable hydrate structure, forcing an in situ swapping of the trapped gas molecules in the structural lattice. In this work, we quantitatively investigate the swapping behavior from injection of pure carbon dioxide and the (CO$_2$ + N$_2$) binary gas mixture through artificial hydrate-bearing sandstone samples by use of a core-flooding experimental apparatus. A total of 13 experimental runs were performed to examine the influence of operating conditions on methane production by CO$_2$/(CO$_2$ + N$_2$) injection in the temperature range of 274.15–277.15 K and 7.039–10.107 MPa pressure. Our results show that the use of the (CO$_2$ + N$_2$) binary gas mixture is advantageous compared to the use of pure carbon dioxide in swapping methane from its hydrate phase; the methane recovery efficiency in brine water systems is enhanced relative to pure water systems. The replenishment of a fresh (CO$_2$ + N$_2$) gas mixture into the vapor phase can be considered as an efficient extraction method because 46.32% of methane was displaced from its hydrate phase with the (CO$_2$ + N$_2$) binary gas mixture after 341.75 h of exposure to the (CO$_2$ + N$_2$) gas mixture. During the CH$_4$–(CO$_2$ + N$_2$) swapping process, gas chromatography analysis and calculations demonstrated that nitrogen molecules can take the place of some methane in small hydrate cages, as long as the equilibrium formation pressure of (CO$_2$ + N$_2$) binary gas hydrate is below that of methane hydrate, even though adding nitrogen to carbon dioxide reduces the thermodynamic driving force for the formation of a new hydrate. When other conditions are similar, the methane gas recovery efficiency increases with the increase of the driving force for the swapping process.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources
Authors: Mu, L. (Intern), von Solms, N. (Intern)
Pages: 3338–3347
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Energy & Fuels
Volume: 31
Issue number: 4
ISSN (Print): 0887-0624
Ratings:
BFI (2018): BFI-level 2
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
Modeling of Asphaltene Precipitation from Crude Oil with the Cubic Plus Association Equation of State

In this study, different modeling approaches using the Cubic Plus Association (CPA) equation of state (EoS) are developed to calculate the asphaltene precipitation onset condition and asphaltene yield from degassed crude oil during the addition of n-paraffin. A single model parameter is fitted to calculate the asphaltene onset condition during the addition of different n-paraffin precipitants (n-pentane to n-hexadecane). Three parameters per precipitant are fitted to calculate the asphaltene yield during the addition of the precipitant. The results obtained from the model are compared with the experimental data for eight different crude oils. Results were also obtained for seven crudes using the Perturbed Chain Statistical Associating Fluid Theory (PC-SAFT) EoS based approach described in the literature. The CPA EoS based approaches treat the asphaltene fraction as an associating component whereas the PC-SAFT EoS based approach does not. A comparison between the approaches shows that the CPA EoS based approaches, developed in this work, give more reliable results. The predictions from the PC-SAFT EoS based approach result in behavior that is unphysical: the mole fraction of n-paraffin (at the precipitation onset) and the asphaltene yield do not decrease with the carbon number of n-paraffin. Furthermore, it is shown that the approach, developed in this work, can predict the onset conditions of asphaltene precipitation resulting from a blend of two or more crudes.
Modeling of Shale Gas Adsorption and its Influence on Phase Equilibrium

Natural gas and oil produced from shale accounts for a significant portion in the global production. Due to the large surface area and high organic content in shale formations, adsorption plays a major role in the storage of the hydrocarbons within the rock and their phase equilibrium. This study provides a comparison of several engineering models for gas adsorption in shale based on the recent literature data for pure and binary gases. For pure components, Langmuir, the modified Toth-Langmuir, and the Multicomponent Potential Theory of Adsorption using Dubinin-Radushkevich potential (MPTA-DRA) were compared. The three models show similar deviations lower than 10%. For binary gases, Multicomponent Langmuir (ML), Ideal Adsorbed Solution Theory (IAST) and MPTA were evaluated, where MPTA shows the lowest deviation with
17.9%. Additionally, we presented an analysis of the phase envelope shift under the influence of the capillary pressure and the adsorption film. ML and IAST were used to calculate the adsorption amount whereas MPTA was used to generate artificial adsorption data over large temperature range and for other homologous hydrocarbons to estimate the ML and IAST parameters. The adsorption film thickness was considered in the calculation of the effective capillary radius and the corresponding capillary pressure. The combined effects modify the saturation pressure in the whole temperature range except at the critical point. The biggest impact was found on the bubble point branch away from the critical point where the interfacial tension of the system is more pronounced.

**General information**

State: Accepted/In press  
Organisations: Department of Chemistry, CERE – Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering  
Authors: Sandoval Lemus, D. R. (Intern), Yan, W. (Intern), Michelsen, M. L. (Intern), Stenby, E. H. (Intern)  
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Modeling Study of High Pressure and High Temperature Reservoir Fluids

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 on 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 VE 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 m3. 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.

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Modeling the influence of potassium content and heating rate on biomass pyrolysis
This study presents a combined kinetic and particle model that describes the effect of potassium and heating rate during the fast pyrolysis of woody and herbaceous biomass. The model calculates the mass loss rate, over a wide range of operating conditions relevant to suspension firing. The shrinking particle model considers internal and external heat transfer limitations and incorporates catalytic effects of potassium on the product yields. Modeling parameters were tuned with experimentally determined char yields at high heating rates (>200 K s⁻¹) using a wire mesh reactor, a single particle burner, and a drop tube reactor. The experimental data demonstrated that heating rate and potassium content have significant effects on the char yield. The importance of shrinkage on the devolatilization time becomes greater with increasing particle size, but showed little influence on the char yields.

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Operating considerations of ultrafiltration in enzyme enhanced carbon capture

Today, enzyme enhanced carbon capture and storage (CCS) is gaining interest, since it can enable the use of energy efficient solvents, and thus potentially reduce the carbon footprint of CCS. However, a limitation of this technology is the high temperatures encountered in the stripper column, which can deactivate the enzymes. One solution to this challenge is the use of ultrafiltration to retain the enzyme in the absorber unit. In this report, a base case of a CCS facility is used to model the impact of such membranes for use in a full scale CCS commercial plant. The base case has an approximate capture capacity of 1 MTonn CO2/year, and is here operated for one year continuously. This publication compares soluble enzymes dissolved in a capture solvent with and without the use of ultrafiltration membranes. The membranes used here have an enzyme retention of 90%, 99% and 99.9%. Enzyme retention is the amount of enzyme that is retained in the absorption column in each cycle. These membranes were modeled with five stripper temperatures 60 °C, 70 °C, 80 °C, 90 °C and above 100 °C. Enzyme deactivation follows a 1st order rate and increases with increasing temperatures. It was found that for all stripper temperatures used in this model, deactivation rates were too high for continuous operation over 1 year, without adding additional enzyme, if an activity of at least 50% should be maintained. With increasing stripper temperatures the membrane retention requirement increased. To retain over 50% activity over a whole year at 70 °C stripper temperature required a membrane of 90% or higher enzyme retention, at stripper temperatures of 90 °C a membrane of 99.9% retention was required for the same result. Finally, it was investigated if stripper temperatures over 100 °C, where instant deactivation was modeled could be used. It was found that with enzyme retention of 99.9%, with instant deactivation, after 1 month 50% of the activity is lost. Thus the use of membranes in enzyme enhanced CCS might be restricted to temperatures below 100 °C, or temperatures the enzyme can withstand for shorter time periods.
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.
Pilot absorption experiments with carbonic anhydrase enhanced MDEA

Mass transfer experiments were carried out on DTU's pilot absorber unit, a 10 m high column packed with 250 Y Mellapak structured packing. The influence of temperature, solvent loading, column height and liquid flow rates on absorption performance were determined for a 30 wt% N-methyl-diethanolamine (MDEA) solvent, with and without the enzyme carbonic anhydrase (CA). The absorption experiments were performed at atmospheric pressure and a gas phase carbon dioxide mole fraction of 0.13. During experiments liquid samples were withdrawn at each meter of column height and the solvent loading was determined by both a density method and the BaCl2 method. After the solvent was loaded to equilibrium it was heated up and reintroduced into the column, where CO2 was stripped off using air as stripping gas. The addition of CA increased the mass transfer significantly in all experiments. Lower absorption temperatures resulted in higher mass transfer in absorption, when 28 and 40 ºC inlet temperature were chosen. The absorption performance decreased with lower solvent flow. The enzyme was also capable of enhancing the desorption process, where higher desorption rates were measured at 45 and 50 ºC with CA enhanced solvent compared to 55 ºC without CA.

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Practical enhancement factor model based on GM for multiple parallel reactions: Piperazine (PZ) CO₂ capture

Reactive absorption is a key process for gas separation and purification and it is the main technology for CO₂ capture. Thus, reliable and simple mathematical models for mass transfer rate calculation are essential. Models which apply to parallel interacting and non-interacting reactions, for all industrially relevant reaction regimes must be developed and validated against experimental measurements. In a previous work, we presented the general model (GM) enhancement factor model for (m+n)-th order reversible reactions and validated it against the numerical solution of the two-film model for absorption, desorption and pinch conditions. In this work, we apply the GM model to multiple parallel reactions. We deduce the model for piperazine (PZ) CO₂ capture and we validate it against wetted-wall column measurements using 2, 5 and 8 molal PZ for temperatures between 40 °C and 100 °C and CO₂ loadings between 0.23 and 0.41 mol CO₂/2 mol PZ. We show that overall second order kinetics describes well the reaction between CO₂ and PZ accounting for the carbamate and bicarbamate reactions. Here we prove the GM model for piperazine and MEA but we expect that this practical approach is applicable for various amines, blends of amines and promoted amines with similar kinetics. We believe that this practical implementation of mass transfer rate calculation will be in the accuracy range of a wetted wall column experiment for other parallel reaction systems. This is in line with our observation from other similar solvents studied, not shown here. Furthermore, we compare the GM model and the numerical solution of the complete two-film model predictions to MEA wetted-wall data and we prove that it is safe to assume that GM and the two-film model give practically identical results. We demonstrate that the expected predictability of CO₂ mass transfer rates using off-the-shelf correlations generally is ±20%.
Prediction of Gas Injection Effect on Asphaltene Precipitation Onset Using the Cubic and Cubic-Plus-Association Equations of State

Gas injection is a proven enhanced oil recovery technique. The gas injection changes the reservoir oil composition, temperature, and pressure conditions, which may result in asphaltene precipitation. In this work, we have used a modeling approach from the literature in order to predict asphaltene precipitation onset condition during gas injection. The modeling approach is used with the Soave Redlich Kwong, Soave Redlich Kwong-Plus-Huron Vidal mixing rule and cubic-plus-association (CPA) equations of state (EoS). Six different reservoir fluids are studied with respect to asphaltene onset precipitation during nitrogen, hydrocarbon gas mixture, and carbon dioxide injection. It is also shown how to extend the modeling approach when the reservoir fluid is split into multiple pseudocomponents. It is observed that the modeling approach using any of the three models can predict the gas injection effect on asphaltene onset conditions. The CPA EoS is more reliable than the other two models, which are sensitive to asphaltene molecular weight and sometimes predict highly nonlinear behavior outside the experimental temperature range used for fitting the model parameters.

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Property Model-Based Chemical Substitution and Chemical Formulation Design

Chemical-based products including structured product formulations and single molecule products have proven to be a boon to mankind and have been a significant part of our economies. Our life and the changes around us cannot be imagined without the presence or involvement of chemicals. But like every coin has two sides, some chemicals constituting these products can also be a curse. This is primarily due to the hazardous environment-related properties that some of these chemicals possess and there are many more chemicals which have not been evaluated due to lack of resources for rigorous, experimental-based estimation methods [1]. Hence, there is a dire necessity to identify such chemicals which may be dangerous to the environment, toxic to human health and harmful for our fragile eco-system.

Besides, in many cases, their corresponding chemical production processes generate harmful emissions, which also have severe impacts on the environment. The concern about the environment and human health has given rise to the REACH regulation implemented by the European Chemical Agency (ECHA), which compels European chemical companies to stop the use of hazardous substances and replace them with environmentally benign chemicals. Additionally, the decisions taken during chemical product design also have an impact on the process and product performance and are influenced by
Prospects of the use of nanofluids as working fluids for organic Rankine cycle power systems

The search of novel working fluids for organic Rankine cycle power systems is driven by the recent regulations imposing additional phase-out schedules for substances with adverse environmental characteristics. Recently, nanofluids (i.e. colloidal suspensions of nanoparticles in fluids) have been suggested as potential working fluids for organic Rankine cycle power systems due to their enhanced thermal properties, potentially giving advantages with respect to the design of the components and the cycle performance. Nevertheless, a number of challenges concerning the use of nanofluids must be investigated prior to their practical use. Among other things, the trade-off between enhanced heat transfer and increased pressure drop in heat exchangers, and the impact of the nanoparticles on the working fluid thermophysical properties, must be carefully analyzed. This paper is aimed at evaluating the prospects of using nanofluids as working fluids for organic Rankine cycle power systems. As a preliminary study, nanofluids consisting of a homogenous and stable mixture of different nanoparticles types and a selected organic fluid are simulated on a case study organic Rankine cycle unit for waste heat recovery. The impact of the nanoparticle type and concentration on the heat exchangers size, with respect to the reference-case, is analyzed. The results indicate that the heat exchanger area requirements in the boiler decrease around 4 % for a nanoparticle volume concentration of 1 %, without significant differences among nanoparticle types. The pressure drop in the boiler increases up to 18 % for the same nanoparticle concentration, but this is not found to impact negatively the pump power consumption.
Publisher's Note to Modeling the influence of potassium content and heating rate on biomass pyrolysis [Appl. Energy J. 194 (2017) 199–211]

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Rate-based modelling and validation of a pilot absorber using MDEA enhanced with carbonic anhydrase (CA)

The great paradox of the 21st century is that we must meet the increasing global demand for energy and products while simultaneously mitigating the climate change. If both these criteria are to be met, carbon capture and storage is an imperative technology for sustainable energy infrastructure development. Post-combustion capture is a mature capture
technology, however, to make it economically attractive, design of innovative solvents and process optimization is of crucial importance. An example for promising solvent is MDEA enhanced with carbonic anhydrase (CA), due to its fast kinetics and low solvent-regeneration energy demand. The focus of this work is to develop a rate-based model for CO₂ absorption using MDEA enhanced with CA and to validate it against pilot-scale absorption experiments. In this work, we compare model predictions to measured temperature and CO₂ concentration profiles for different L/G ratios, lean CO₂ loadings, gas CO₂ content and packing height. We show that the developed model is suitable for CO₂ capture simulation and optimization using MDEA and MDEA enhanced with CA. Furthermore, we investigate the accuracy of the General Method (GM) enhancement factor model for CO₂ absorption/desorption using wetted-wall column data: 0 to 0.5 CO₂ loading and temperatures between 298 and 328 K. The present study represents a first step towards developing and optimizing a CA promoted MDEA CO₂ capture process.

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**Simultaneous Description of Activity Coefficients and Solubility with eCPA**

In the many developments of electrolyte equations of state presented over the past decades, several different properties have been in focus. A property that has not been widely used as a fitting property is salt solubility. This work presents a
new parametrization of the eCPA equation of state with salt specific parameters. The focus is on accurate description of the salt solubility, and low deviation correlations are obtained for all salts investigated. The inclusion of the solubility data in the parametrization has, compared to parameters only parametrized to osmotic coefficients and activity coefficients, not significantly affected the deviations of the osmotic coefficients and activity coefficients. The average deviations of the activity coefficient does increase slightly and it was found that the increase in deviations was almost entirely due to reduced accuracy at high temperature and high molality. The model is, furthermore, compared to the activity coefficient model, Extended UNIQUAC. It is shown that the eCPA provides more accurate solubility description at higher temperatures than Extended UNIQUAC but also that Extended UNIQUAC is slightly better at describing the activity coefficients. Overall the two models perform similarly.
Solubility Modeling of the Systems Ni(NO₃)₂·H₂O and Fe(NO₃)₃·Ni(NO₃)₂·H₂O with the Extended Universal Quasichemical (UNIQUAC) Model

Thermodynamic modeling of the binary systems Ni(NO₃)₂·H₂O and Ni(NO₃)₂·H₂O and of the ternary system of Fe(NO₃)₃·Ni(NO₃)₂·H₂O along the 30 °C isotherm are presented. The extended UNIQUAC model was applied for the thermodynamic assessment of the investigated systems, the model parameters were regressed simultaneously using the available databank but with additional experimental data recently published in the open literature. A revision for previously published parameters for the nickel ion, new parameters for the iron(III) nitrate system, and interaction parameters for the Ni²⁺–Fe³⁺ interaction are presented. Based on this set of parameters, the equilibrium constants of hydrates were determined. The model represents the experimental data with good accuracy from the freezing point region to the boiling points of the solutions.

General information
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Organisations: Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering, University Hassan I
Authors: Arrad, M. (Ekstern), Kaddami, M. (Ekstern), El Goundali, B. (Ekstern), Thomsen, K. (Intern)
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Web of Science (2015): Indexed yes
Thermodynamic Analysis of Chalk–Brine–Oil Interactions

The surface complexation models (SCMs) are used successfully for describing the thermodynamic equilibrium between the pure calcite surface (carbonate and calcium sites) and brine solutions. In this work, we show that the model parameters that are reported for the calcite–brine system are not applicable to the natural carbonates. We adjust the SCM reaction equilibrium constants by fitting the model to the zeta potential data that are reported for the pulverized Stevns Klint chalk. Then, we use the model, implemented in the PhreeqcRM geochemistry package coupled with a finite volume solver, to predict the breakthrough composition of different ions in the chromatographic experiments on the intact Stevns Klint chalk cores. Again, the model falls short in predicting the reactive transport of brine in a natural carbonate, implying that zeta potential data is not enough for optimizing the SCM model parameters for the reactive transport applications. We propose an optimization procedure that fits the coupled SCM–transport model parameters to the chromatographic (single-phase core flooding) data. The zeta potential measurements are implemented in the optimization scheme as nonlinear constraints. We then use the optimized model to study the thermodynamic equilibrium between the oil and chalk surfaces in the presence of different brine compositions, including the dissolution and precipitation of minerals. We represent the chalk–oil interactions by acid–base equilibrium reactions between the calcium and carbonate sites on the chalk surface and carboxylic acids and amine bases on the oil surface, respectively. Comparing the model results to a data set of the spontaneous imbibition experiments for chalk shows that the remaining oil saturation in the imbibition experiments is correlated with the number of bonds between the amine and carboxylate groups on the oil surface and the carbonate and protonated calcium on the chalk surface.

General information

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Organisations: Centre for oil and gas – DTU, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering, Department of Chemistry
Thermodynamic modelling of acid gas removal from natural gas using the Extended UNIQUAC model

Thermodynamics of natural gas sweetening process needs to be known for proper design of natural gas treating plants. Absorption with aqueous N-Methyldiethanolamine is currently the most commonly used process for removal of acid gas (CO₂ and H₂S) impurities from natural gas. Model parameters for the Extended UNIQUAC model have already been determined by the same authors to calculate single acid gas solubility in aqueous MDEA. In this study, the model is further extended to estimate solubility of CO₂ and H₂S and their mixture in aqueous MDEA at high pressures with methane as a makeup gas.

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Organisations: Department of Chemical and Biochemical Engineering, Department of Chemistry, CERE – Center for Energy Resources Engineering
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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
Towards the understanding of microbial metabolism in relation to microbial enhanced oil recovery

In this study, Bacillus licheniformis 421 was used as a model organism to understand the effects of microbial cell growth and metabolite production under anaerobic conditions in relation to microbial enhanced oil recovery. The bacterium was able to grow anaerobically on different carbon compounds, where n-alkanes were preferred over molasses as carbon source. The bacterium grew slowly when n-alkanes were used as carbon source, however, formation of emulsions and reduction of interfacial tension (IFT) were still observed. The bacterial cells were mainly present at the interface of the synthetic seawater medium and the n-alkanes. The bacterium produced lipopeptide lichenysin G which was detected both in the water and in the emulsion phase. We propose that the bacterial cells themselves or metabolites attached to the cell surface are the main players in the formation of emulsions and IFT reduction.
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 (N-methyl-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.

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Engineering, Center for Energy Resources Engineering, KT Consortium, PROSYS - Process and Systems Engineering
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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**

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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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BFI (2008): BFI-level 1
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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 density gradient theory based method for surface tension calculations

The density gradient theory has been becoming a widely used framework for calculating surface tension, within which the same equation of state is used for the interface and bulk phases, because it is a theoretically sound, consistent and computationally affordable approach. Based on the observation that the optimal density path from the geometric mean density gradient theory passes the saddle point of the tangent plane distance to the bulk phases, we propose to estimate surface tension with an approximate density path profile that goes through this saddle point. The linear density gradient
theory, which assumes linearly distributed densities between the two bulk phases, has also been investigated. Numerical problems do not occur with these density path profiles. These two approximation methods together with the full density gradient theory have been used to calculate the surface tension of various systems, from non-polar binary mixtures to complex multicomponent associating fluids, combined with the Peng-Robinson and the Cubic Plus Association equations of state. From an overall point of view, the approximation method with the density path profile passing the saddle point and the full density gradient theory offer comparable performance in predicting surface tension, while the linear density gradient theory frequently overpredicts. Limitations have been seen for all the three methods in correlating the surface tension of particular systems, with a single adjustable parameter for the cross influence parameter.

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Organisations: Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources
Authors: Liang, X. (Intern), Michelsen, M. L. (Intern), Kontogeorgis, G. (Intern)
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Scopus rating (2012): SJR 1.152 SNIP 1.286 CiteScore 2.31
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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.

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Organisations: Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering, Politecnico di Milano
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Application of various water soluble polymers in gas hydrate inhibition

Formation of hydrates in gas transmission lines due to high pressures and low temperatures is a serious problem in the oil and gas industry with potential hazards and/or economic losses. Kinetic hydrate inhibitors are water soluble polymeric compounds that prevent or delay hydrate formation. This review presents the various types of water soluble polymers used for hydrate inhibition, including conventional and novel polymeric inhibitors along with their limitations. The review covers the relevant properties of vinyl lactam, amide, dendrimeric, fluorinated, and natural biodegradable polymers. The factors affecting the performance of these polymers and the structure-property relationships are reviewed. A comprehensive review of the techniques used to evaluate the performance of the polymeric inhibitors is given. This review also addresses recent developments, current and future challenges, and field applications of a range of polymeric kinetic hydrate inhibitors.

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In this study the effect of carbonic anhydrase addition on the absorption of CO₂ was investigated in a wetted wall column apparatus. Four different solvents: MEA (a primary amine), AMP (a sterically hindered primary amine), MDEA (a tertiary amine) and K₂CO₃ a carbonate salt solution were tested in concentrations from 5 to 50 wt%. Necessary mass transfer parameters such as liquid side mass transfer coefficient and solvent and enzyme reaction rates were determined in a temperature range from 298 to 328 K and benchmarked to a 30 wt% MEA solution.

The study reveals that the addition of the enzyme carbonic anhydrase (CA) dramatically increases the liquid side mass transfer coefficient for 30 wt% MDEA and 15 wt% K₂CO₃. 30 wt% AMP has a moderate increase whereas 30 wt% MEA was unchanged. The results confirm that bicarbonate forming solvent which do not produce carbamate benefit from CA.

The results reveal the impact of temperature in relation to CA. A temperature increase resulted in lower liquid side mass transfer rate for 30 wt% MDEA and 15 wt% K₂CO₃ but in higher rate for 30 wt% AMP. The overall first order enzyme reaction rate (s⁻¹) was linearly dependent on enzyme concentration for 30 wt% MDEA and 15 wt% K₂CO₃ at 313 K. The derived enzymatic reaction rate constant kenz (m³ kg⁻¹ s⁻¹) for 15 wt% K₂CO₃ at 313 K was about 9 times higher than for 30 wt% MDEA and 10 times higher than for 30 wt% AMP. Temperature and concentration did not observably influence the enzymatic rate constant in the concentration range of 5 to 15 wt% K₂CO₃. The higher solvent concentration only led to a slightly higher reaction rate. A solution with 20 wt% K₂CO₃ had almost 3 times higher enzyme reaction rate compared to 15 wt% at 298 K and increased with temperature to almost 5 times faster at 328 K. The enzymatic reaction rate for MDEA decreased with both temperature and solvent concentration from 15 to 30 wt%. An increase to 50 wt% resulted in a decrease in reaction rate due to less water present.

Pilot plant campaigns were carried out for different solvents and conditions and the results were successfully modelled using intrinsic data obtained from the wetted-wall column experiments.
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.
CO₂ Capture Dynamic and Steady-State Model Development, Optimization and Control: Applied to Piperazine and Enzyme Promoted MEA/MDEA

Despite the efforts and recent advances in renewable energy sources, the energy infrastructure is not yet ready to replace the fossil-fuel fired power plants with renewables. Thermal power plants represent the main energy supply and especially in developing countries, they are expected to dominate the market in the coming decades. However, the growing focus on mitigation of anthropogenic CO₂ requires integration of fossil-fuel fired power plant with CO₂ capture units. Post-combustion capture is the most mature capture technology and it is suitable for various processes in power plants, steel industry, cement production, and bio-chemical industry. However, to make CO₂ capture economically attractive, design of innovative solvents, optimization of operation conditions/process configuration and operational flexibility are of crucial importance.

This thesis aims to contribute to the development of efficient CO₂ post-combustion capture technology using alkanolamine solvents. Amine based CO₂ post-combustion capture is a reactive absorption process which implies complex mechanism of simultaneously occurring reaction and mass transport phenomena. Accordingly, first a simplified and easy to implement but general valid mass transfer model is developed and applied to single and parallel reactions systems, i.e. MEA, PZ and CA/MDEA. This mass transfer model uses existing correlations for mass and hydraulic characteristic and an enhancement factor to describe the acceleration of the mass transfer rate due to the reaction between CO₂ and amines. Afterwards, this sub-model together with the extended UNIQUAC thermodynamic model and correlations for physical properties is incorporated in a rate-based model for CO₂ absorption and desorption. The developed model is applied to MEA, PZ, PZ/K₂CO₃ and CA/MDEA and it is benchmarked against experimental pilot plant data and various models from independent research groups.

The validated steady-state model is used to determine set of optimal operation parameters for CO₂ capture post-combustion capture using PZ. This study accounts for the solubility window of PZ when determining the optimal and feasible operating conditions. The results are created in Aspen Plus using the hybrid CAPCO₂ rate-based user model. This model considers slurry formation in the calculation of CO₂ mass transfer rate. 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 molal 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.

Furthermore, this thesis presents a dynamic rate-based model for CO₂ absorption and desorption using MEA and PZ as solvent. This dynamic model is an extension of the steady-state model as it uses the same thermodynamic-, mass transfer-, kinetic- and physical property- modules. These modules are implemented in Fortran and interfaced with the dynamic model which is implemented in Matlab. The developed model is used to investigate the transient behavior of a post-combustion plant using MEA and PZ. Moreover, a proportional-integral control structure is developed to investigate the controllability of the PZ based post-combustion plant compared to the MEA plant. The results reveal that PZ may be a better solvent than MEA as it can accommodate disturbances with less variability in the manipulated variables. However, control design alternatives and/or model based control structure should be developed to reduce the long settling time of the PZ plant compared to the MEA plant.
Energy production and transportation is responsible for more than 60% of our CO2 emission. In particular coal-fired power plants are big contributors. However, these large scale facilities offer the possibility to effective CO2 capture through post-combustion processes. There are several options for such CO2 capture. The problem is to make the absorption/desorption processes energetically and thereby economically viable. One process under investigation involves alkanoamines as absorbents in aqueous solutions. In these systems CO2 is captured either by carbonate and/or carbamate formation. We have studied the 2-amino-2-methyl-1-propanol (AMP) and the AMP-water phase diagram and its ability for CO2 capture. The first crystal structure in the AMP-water system has been solved from powder diffraction data: AMP trihydrate (triclinic, P-1, a = 6.5897(3), b = 6.399 (2), c = 6.3399(2) Å and α = 92.40 (3), β = 113.345(3) and γ = 94.06 (2)°). In the AMP-water CO2 system two structures, a carbamate, AMPH-AMPCO2 and a carbonate, (AMPH)2-CO3 are known [1]. In this work we solved a new structure from powder diffraction data, AMPH-HCO3 hydrate (monoclinic, I2/a, a = 21.8522( ), b = 6.2149(15), c = 12.1300(3) Å, β = 104.036(16)°) readily formed when using <40 at% AMP in water.

Density and phase equilibrium of the binary system methane + n-decane under high temperatures and pressures
Densities of the binary system methane + n-decane have been determined through a vibrating tube densitometer from (278.15-463.15) K at pressures up to 140 MPa, and for methane mole fractions up to 0.8496. Negative excess volumes were found under the experimental conditions studied. Moreover isothermal compressibility values were obtained by differentiation from the Tammann-Tait correlation of the determined density values. Isobaric thermal expansion coefficients were also calculated based on differentiation from the isobaric fit of density data. We also measured the phase equilibrium of this binary system by using a variable volume cell with full visibility from (293.15-472.47) K for three mixtures with methane mole fractions of 0.4031, 0.6021 and 0.8496. Liquid fraction upon expansion below the saturation pressure has also been determined. Finally different equations of state were used to calculate the experimental density and excess volume data as well as the phase envelope data. No direct regression of the experimental data was involved in most of the calculation in order to provide a fair comparison of the performance of different models.
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).

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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].
Dynamic simulation and analysis of a pilot-scale CO2 post-combustion capture unit using piperazine and MEA

Post-combustion capture is a promising technology for developing CO2 neutral power plants. However, to make it economically and technically feasible, capture plants must follow the fast and large load changes of the power plants without decreasing the overall performance of the plant. Dynamic modeling and simulation is therefore needed to evaluate the performance of this plant under critical operation.

In this work, we evaluate the transient response of an absorber and a desorber for step changes of key process parameters, e.g. flue gas flow and composition, lean and rich CO2 loading, etc. We show the results for the baseline 30 wt% MEA and the low energy piperazine (PZ) solutions. This analysis reveals that the absorber reaches steady-state faster using MEA compared to PZ. This is related to the shift of the mass transfer zone due to changes in temperature. The transient operation in the regeneration unit is somewhat similar while using both solvents: an initial fast decrease of the lean loading is followed by a slow transient period as the system approaches steady-state conditions. We show the presence of inverse response in the stripper column when the rich loading decreases or the feed's temperature reduces using PZ solvent. Thus, we demonstrate that the dynamics of the MEA system cannot be extrapolated to other solvents.

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Enhanced Oil Recovery with Application of Enzymes

Enzymes have recently been reported as effective enhanced oil recovery (EOR) agents. Both laboratory and field tests demonstrated significant increase in the ultimate oil production. Up to 16% of additional oil was produced in the laboratory conditions and up to 269 barrels of additional oil per day were recovered in the field applications. The following mechanisms were claimed to be responsible for the enhancement of the oil production due to enzymes: wettability improvement of the rock surface; formation of the emulsions; reduction of oil viscosity; and removal of high molecular weight paraffins. However, the positive effect of enzymes on oil recovery is not that obvious. In most of the studies commercial enzyme products composed of enzymes, surfactants and stabilisers were used. Application of such samples makes it difficult to assign a positive EOR effect to a certain compound, as several components of commercial mixture might possess surface-active properties. Hence, the main goals of the present study were to establish whether enzymes alone can improve oil production and to identify mechanisms that might underlie enzymatic EOR (EEOR), especially, under conditions of the North Sea petroleum reservoirs.

At the first stage of the work enzyme samples that might have potential for EOR applications were selected. Wettability tests such as measurements of contact angles and determination of adhesion behaviour were applied as screening tools. The group of lipases/esterases demonstrated strong ability to detach oil from the calcite surface and was identified as the most promising group for further investigations. Wettability improvement due to protein adsorption on to the mineral was proposed as the main mechanism for EEOR. It was also proved that the enzyme molecules themselves caused change of the wetting state of calcite, while presence of stabilising ingredients did not interfere the results. Implementation of such a mechanism of enzymatic action under reservoir conditions might be limited by retention of the protein molecules in the porous medium. In order to verify this hypothesis, adsorption behaviour of enzymes/proteins on the reservoir rocks was studied by application of the static adhesion tests and adsorption experiments on powders, as well as of dynamic flow-through experiments. It was established that enzymes are indeed significantly lost during the transport in the porous media due to the irreversible adsorption. The adsorption capacity of carbonate material was found to be much higher compared to sandstone. Various methods (forexample, change of ionic strength and pH of the enzyme...
solution and displacing fluid) were applied in order to desorb attached protein molecules, but no desorption was observed. Another possible mechanism that might underlie EEOR is formation of enzyme-stabilised emulsions. Similar to the wettability screening, lipases/esterases demonstrated the best surface active properties: they formed the most stable emulsions with rather small drops. Light fractions of the crude oil participated mostly in formation of the protein-stabilised emulsions. Incubation of the oil-[enzyme + sea water] systems was found to be important in order to obtain high stability of emulsions. Combined application of enzymes and solid particles was an alternative way to increase emulsion stability. Other crude oil-brine interaction tests revealed additional problems that can arise during the application of enzymatic EOR. Interaction of the enzyme solution with the crude oil can induce gelation/emulsification of the propylene glycol (the main component of the enzyme productstabilisers). Moreover, when purified enzyme containing almost no stabilisers was used, a highly viscous oil-in-water emulsion was formed. Finally, assessment of enzymes as EOR agents under conditions similar to the conditions of the petroleum reservoirs was carried out in core flooding experiments. Two types of enzymes (lipase and amylase) were selected based on the results from the wettability and emulsion studies. They were only tested in tertiary mode, employing various injection schemes. Application of enzymes in sandstone core samples resulted in increase of the ultimate oil production by 0.23-1.69% relative to original oil in place, while no additional oil due to enzymes was produced from chalk. Wettability change was confirmed to be the main EOR mechanism, while emulsification plays less significant role. Overall, enzymes have possessed low potential for EOR applications at least in sandstone and chalk reservoirs containing light crude oils. An alternative technique that will shift adsorption balance towards reversible adsorption should be established in order to make enzymatic EOR an effective and economically feasible oil recovery method.

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Enzymes in CO2 Capture
The enzyme Carbonic Anhydrase (CA) can accelerate the absorption rate of CO2 into aqueous solutions by several-fold. It exist in almost all living organisms and catalyses different important processes like CO2 transport, respiration and the acid-base balances. A new technology in the field of carbon capture is the application of enzymes for acceleration of typically slow ternary amines or inorganic carbonates. There is a hidden potential to revive currently infeasible amines which have an interesting low energy consumption for regeneration but too slow kinetics for viable CO2 capture. The aim of this work is to discuss the measurements of kinetic properties for CA promoted CO2 capture solvent systems. The development of a rate-based model for enzymes will be discussed showing the principles of implementation and the results on using a well-known ternary amine for CO2 capture. Conclusions will be drawn revealing basic unexpected process conditions which are beneficial to enzyme promoted amines like water presence, temperatures, and similar basic variables.

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Evaluation of the Cubic-Plus-Association Equation of State for Ternary, Quaternary, and Multicomponent Systems in the Presence of Monoethylene Glycol

Dew point specifications are of high interest in the natural gas industry. The CPA equation of state (EoS) was previously validated against both water content and phase equilibrium data. Moreover, solid model parameters were estimated for four natural gas main components (methane, ethane, propane, and carbon dioxide). In this study we have extended the use of CPA EoS to perform equilibrium temperature calculations for natural gas main components with (mono-)ethylene glycol (MEG) as an inhibitor. The ternary systems with aqueous MEG solution include methane, ethane, propane, carbon dioxide, and hydrogen sulfide. The quaternary systems with aqueous MEG solution include methane + ethane, methane + propane, methane + n-heptane, and methane + n-octane. Three multicomponent systems (>4 components) were also studied. The temperature range of the literature data is between 241.25–333.15 K, and the pressure range is between 0.1–24.8 MPa. The results in all cases are compared against experimental data, and very good agreement with experimental data is obtained.

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Fast pyrolysis of biomass at high temperatures

This Ph.D. thesis describes experimental and modeling investigations of fast high temperature pyrolysis of biomass. Suspension firing of biomass is widely used for power generation and has been considered as an important step in reduction of greenhouse gas emissions by using less fossil fuels. Fast pyrolysis at high temperatures plays a significant role in the overall combustion process since the biomass type, the reaction kinetics and heat transfer rates during pyrolysis influence the volatile gas release. The solid residue yield and its properties in suspension firing, including particle size and shape, composition, reactivity and burnout depend significantly on the operating conditions of the fast pyrolysis. Biomass fast pyrolysis experiments were performed in a laboratory-scale wire mesh reactor and bench scale atmospheric pressure drop tube / entrained flow reactors with the aim to investigate the effects of operating parameters and biomass types on yields of char and soot, their chemistry and morphology as well as their reactivity using thermogravimetric analysis. The experimental study was focused on the influence of a wide range of operating parameters including heat treatment temperature, heating rate, particle size, residence time, inorganic matter and major organic biomass compounds. Woody and herbaceous biomass were used as fuels. Char yields from the drop tube and entrained flow reactors were lower than those obtained in the wire mesh reactor, emphasizing the importance of heating rate on the product yields. The char yield decreased significantly between 10 and 600K s⁻¹, but continued to decrease with increasing heating rate, and was lowest for the drop tube / entrained flow reactors with estimated heating rate of > 10⁴ K s⁻¹. The heat treatment temperature and potassium content affected the char yield stronger than the heating rates and differences in the plant cell wall compounds between 600 and 3000K s⁻¹. The heat treatment temperature affected more the herbaceous biomass char yield compared with wood.

The differences in the char yield for particle size fractions in the range of 0.05mm were negligible, leading to the conclusion that the biomass particle can be assumed isothermal, when its size did not exceed 0.425 mm. Compared to smaller particles, the larger pinewood particles(dₜ > 0.85 mm) required more than 1 s holding time for the complete conversion at intermediate and fast heating rates. The influence of heating rate on the char yields was less pronounced for larger particles (from 0.85 to 4 mm) obtained at temperatures > 1250°C in the wire mesh reactor, single particle burner and drop tube reactor, due to the predominance of internal heat transfer control within the large particles. Potassium compared to all other ash elements in the fuels had the highest influence on the char yield. The effect of potassium on the char yield was stronger at low and intermediate heating rates where potassium catalyzed the repolymerization and cross-linking reactions, leading to higher char yields. Silicon compounds abundant in herbaceous biomass had a negligible influence on the char yield and reactivity. However, a very high content of silicon oxides in biomass (> 50% of the overall biomass inorganic matter) significantly affected the char morphology, as observed for rice husk. For this fuel, the high content of low-temperature melting amorphous silicon oxidesled to the formation of a glassy
shell on rice husk chars at 1000-1500°C. The ability of char to melt in fast pyrolysis followed the order pinewood > beechwood, straw > rice husk, and was related to the formation of metaplast. Different particle shapes of beechwood and leached wheat straw chars produced in the drop tube reactor which have similar potassium content suggested a stronger influence of the major biomass cell wall compounds (cellulose, hemicellulose, lignin and extractives) and silicates on the char morphology than alkali metals. In this study, potassium lean pinewood (0.06 wt. %) produced the highest soot yield (9 and 7 wt. %) at 1250 and 1400°C, whereas leached wheat straw with the higher potassium content (0.3 wt. %) generated the lowest soot yield (2 and 1 wt. %). Soot yields of wheat and alfalfa straw at both temperatures were 5% points lower than wood soot yields and 3% points higher than leached wheat straw soot yield, indicating that potassium plays a minor role on the soot formation. The leaching of alkali from wheat straw additionally resulted in a removal of lignin, leading to the decreased formation of polycyclic aromatic hydrocarbon precursors, and thereby to lower soot yields. Pinewood soot particles generated at 1250°C were significantly larger (77.7 nm) than soot particles produced in pinewood (47.8 nm) pyrolysis at 1400°C, beechwood (43 nm) and wheat straw (30.8 nm) devolatilization at both temperatures. The larger pinewood soot particles were related to the formation of tar balls known from smoldering combustion. The major difference in nanostructure of pinewood, beechwood and wheat straw soot was in the formation of multi and single core particles. Pinewood soot particles generated at 1250°C were mainly multi core structures compared to pinewood soot generated at 1400°C, combining both single and multi core particles. Beechwood and wheat straw soot samples had multi and single core particles at both temperatures. In thermogravimetric analysis, the maximal reaction rate of pinewood soot was shifted to temperatures about 100°C higher than for the other samples in both oxidation and CO2 gasification, indicating a significantly lower reactivity. Soot samples produced at 1400°C were more reactive than soot generated at 1250°C. The beechwood and wheat straw soot samples were more graphitic than pinewood soot based on the electron energy loss spectroscopy (EELS) analysis. In contrast to expectations of graphitic structures to react slower than amorphous samples, beechwood and wheat straw soot were 35 and 571 times more reactive than pinewood soot prepared at 1400°C. The presence of potassium in wheat straw soot mainly as water-soluble KCl, KOH, KHCO3 and K2CO3 to a minor extent bonded to the soot matrix in oxygen-containing surface groups (e.g., carboxyl, phenol) or intercalated in soot graphene layers led to a higher reactivity in CO2 gasification compared to low-alkali containing pinewood soot. The results showed that potassium has a dominating effect on the soot reactivity compared to nanostructure and particle size. A mathematical model of biomass fast pyrolysis was developed to predict the gas and char yield of wood and herbaceous biomass at heating rates > 600 K s\(^{-1}\). The model includes both kinetics and external and internal heat transfer assuming that mass transfer is fast. The model relies on the concept applied in fast pyrolysis of cellulose through the formation of an intermediate liquid (so-called metaplast) which reacts further to form char and gas. The kinetics of the fast pyrolysis was described through the Broio-Shafizadeh scheme for biomass. The catalytic effect of potassium which is a major ash element influencing the char yield was included in the model.

**Hydrate equilibrium data for the CO2 + N2 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.
Introduction to Applied Colloid and Surface Chemistry

Colloid and Surface Chemistry is a subject of immense importance and implications both to our everyday life and numerous industrial sectors, ranging from coatings and materials to medicine and biotechnology.

How do detergents really clean? (Why can’t we just use water?) Why is milk “milky” Why can we deliver drugs in better and controlled ways? Coating industries wish to manufacture improved coatings e.g. for providing corrosion resistance, which are also environmentally friendly i.e. less based on organic solvents and if possible exclusively on water. Food companies want to develop healthy, tasty but also long-lasting food products which appeal to the environmental authorities and the consumer. Detergent and enzyme companies are working to develop improved formulations which clean more persistent stains, at lower temperatures and amounts, to the benefit of both the environment and our pocket. Cosmetics is also big business! Creams, lotions and other personal care products are really just complex emulsions.

All of the above can be explained by the principles and methods of colloid and surface chemistry. A course on this topic is truly valuable to chemists, chemical engineers, biologists, material and food scientists and many more.

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).
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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Low immediate scientific yield of the PhD among medical doctors
Background: We studied the scientific yield of the medical PhD program at all Danish Universities.
Methods: We undertook a retrospective observational study. Three PhD schools in Denmark were included in order to evaluate the postdoctoral research production over more than 18 years through individual publications accessed by PubMed.
Results: A total of 2686 PhD-graduates (1995-2013) with a medical background were included according to registries from all PhD schools in Denmark. They had a median age of 35 years (interquartile range (IQR), 32-38) and 53 % were women at the time of graduation. Scientific activity over time was assessed independently of author-rank and inactivity was measured relative to the date of graduation. Factors associated with inactivity were identified using multivariable logistic regression. 88.6 % of the PhD theses were conducted in internal medicine vs. 11.4 % in surgery. During follow-up (median 6.9 years, IQR 3.0-11.7), PubMed data searches identified that 87 (3.4 %) of the PhD graduates had no publication after they graduated from the PhD program, 40 % had 5 or less, and 90 % had 30 or less. The median number of publications per year after PhD graduation was 1.12 (IQR 0.61-1.99) papers per year. About 2/3 of the graduates became inactive after 1 year and approximately 21 % of the graduates remained active during the whole follow-up. Female gender was associated with inactivity: adjusted odds ratio 1.59 (95 % confidence interval 1.24-2.05).
Conclusions: The scientific production of Danish medic PhD-graduates was mainly produced around the time of PhD-graduation. After obtaining the PhD-degree the scientific production declines suggesting that scientific advance fails and resources are not harnessed.

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Authors: Fosbol, E. L. (Ekstern), Fosbel, P. L. (Intern), Rerup, S. (Ekstern), Ostergaard, L. (Ekstern), Ahmed, M. H. (Ekstern), Butt, J. (Ekstern), Davidsen, J. (Ekstern), Shanmuganathan, N. (Ekstern), Juul, S. (Ekstern), Lewinter, C. (Ekstern)
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Measurement of properties and pilot testing. CERE lab and model development

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Mechanics of the Separating Surface for a Two-Phase Co-current Flow in a Porous Medium

A mechanical description of an unsteady two-phase co-current flow in a porous medium is developed based on the analysis of the geometry and motion of the surface separating the two phases. It is demonstrated that the flow should be considered as essentially three-dimensional, even if the phase velocities are co-directed, since the phase interface is on average inclined to the direction of the flow. Kinematics of the flow is described, distinguishing between the average velocities of the bulk phases and their velocity near the interface between them. Dynamics of the flow is analyzed by means of the extended Maxwell-Stefan formalism, as in our previous paper (Shapiro 2015). Force balances are formulated in the directions parallel and orthogonal to the flow. A complete system of the flow equations, generalizing the traditional Buckley–Leverett and Rappoport–Leas system, is derived. Sample computations show that one of the main effects produced by the new system is sharpening of the displacement front, which otherwise would be washed out by the capillary forces, as in the solution of the Rappoport–Leas equation.
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 Asphaltene Onset Precipitation Conditions with Cubic Plus Association (CPA) and Perturbed Chain Statistical Associating Fluid Theory (PC-SAFT) Equations of State

Asphaltene precipitation has been one of the major problems in the oil industry, and its modeling is still believed to be quite a complex issue due to the different characteristics of thousands of heavy components in crude oil. There have been several attempts to model asphaltene precipitation using various equations of state and empirical models. In the past few years, association models based on CPA and SAFT equations of state have been found to be promising models for studies of asphaltene precipitation. In this work, we compare asphaltene precipitation results obtained from different modeling approaches based on CPA, PC-SAFT with association (PC-SAFT (WA)), and PC-SAFT without association (PC-SAFT (WOA)) models. While the modeling approaches for the CPA and PC-SAFT (WOA) have been described before in various literature, the modeling approach for PC-SAFT (WA) is proposed in this work. All three models require the same number of experimental data points (at least three upper onset pressures and one bubble pressure) in order to obtain model parameters. Different types of asphaltene phase behavior for different reservoir fluids, where asphaltene solubility either decreases or increases with temperature, and where asphaltene precipitation occurs during reservoir fluid depressurization, and the effect of gas injection are studied in order to investigate thoroughly the potential and reliability of the models. A total of five reservoir fluids and one model oil are studied with all three models. It is found that the modeling approach with the CPA EoS is more reliable compared to the other two approaches used in this study. The advantage of the association term to describe interactions between asphaltene and other stock tank oil (STO) heavy components is also evident from this study. The sensitivity of SARA data to the modeling approach based on PC-SAFT (WOA) is also analyzed. Finally, the relationship between the binary interaction parameter of the asphaltene-CO$_2$ pair and crossover temperature, below which asphaltene solubility increases in reservoir fluid, with CO$_2$ gas injection is also studied.
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 kij fitted to binary data.

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Organisations: Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering, Statoil ASA
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Modeling systems relevant to the biodiesel production using the CPA equation of state

In this study, CPA parameters for heavy esters, glycerides, organic acids, and glycerol are presented, together with trends of these parameters against the van der Waals volume. Such trends allow the prediction of parameters for compounds for which data are not available. Pure fluid parameters were estimated by adjusting model predictions to recent DIPPR correlations and carefully selected literature data. Then, the performance of CPA was evaluated in correlating the vapor–liquid and liquid–liquid equilibrium of binary systems containing fatty acids and their esters, glycerides, water, alcohols and/or glycerol. Satisfactory correlation results were obtained using one (water-acids, alcohols/water - glycerol) or two (systems containing fatty acid esters with water, alcohols or glycerol and mixtures containing glycerides and alcohols) interaction parameters. Moreover, the interaction parameters show smooth trends with carbon chain length, permitting extrapolation for systems for which data are not available. Finally, the estimated parameters and correlations were used for the prediction of liquid-liquid equilibrium of one ternary and one multicomponent mixture. The results showed that accurate predictions are feasible, however indicated the need of more accurate data, at least for important binary mixtures, such as the systems with glycerol.

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Modelling of Salt Solubilities for Smart Water flooding in Carbonate Reservoirs using Extended UNIQUAC Model

For most oil reservoirs which were drilled with conventional methods, the expected initial recovery of available hydrocarbons maybe as low as 15% – thus leaving 85+% of hydrocarbons in the reservoir. Implementation of mechanical methods including pump jacks and initial gas injection or thermal recovery can increase that capture up to 25-30% of original oil in place (OOIP). But cost effective Enhanced Oil Recovery (EOR) techniques if implemented correctly can be used to produce another 10-15% of the initially available hydrocarbons.

Advanced water flooding (i.e. altering injection brine compositions by varying concentration of selected ions) is an enhanced oil recovery method which in low cost, non-toxic manner increases oil recovery from various carbonate reservoirs. Dan and Halfdan are chalk reservoirs from the Danish North Sea, which are matured oil fields that have been flooded with water for more than a decade and are potential candidates for brine composition based EOR. Advanced water flooding through alteration in brine composition has been termed as Smart Water(SmW) Flooding, Designed Water flooding, Low salinity brine injection, LowSal™ EOR, and Advanced Water flooding in different research studies.

Several spontaneous imbibition and water flooding experiments have been conducted in order to understand the fundamental mechanism behind the observed increase in oil recovery for variation in injection of brine composition. When reported in literature, this observed increase in oil recovery has been explained using the wettability alteration mechanism. The wettability alteration mechanism reported in literature can be divided into two parts:

1. Substitution of calcium by magnesium: When Mg containing brine is injected into a core plug, the existing Ca^{2+} from the mineral surface/lattice is gradually replaced by the injected Mg^{2+}. Decrease in magnesium concentration in the effluent and the corresponding increase in calcium concentration further support this phenomenon.

2. Adsorption of SO_{4}^{2-} ions: When SO_{4}^{2-} ions are injected into the core plugs along with Ca^{2+} and/or Mg^{2+} ions, then SO_{4}^{2-} ions get adsorbed on the mineral surface. This leads to desorption of carboxyl ions from the mineral surface and makes the oil more mobile. Thus, eventually leading to an increase in oil recovery. According to the wettability alteration mechanism, an increase in oil recovery therefore takes place when brines with high concentrations of Ca^{2+}, Mg^{2+}, and SO_{4}^{2-} ions are injected. It has been further recommended that precipitation of ions must be avoided as precipitation can choke the pore throats and thus have an adverse effect on the sweep efficiency of the flooded water. Several questions have been raised to the wettability alteration mechanism due to fundamental contradictions with experiments. It has been observed that Stevns Klint chalk from Denmark shows consistent increase in oil recovery for an increase in injection brine
SO$_4^{2-}$ concentration. But similar increases in oil recovery are not observed for Niobrara or Rørdal outcrop chalk core plugs.

Observed increases in oil recovery for completely water wet core plugs are also contradictory to the proposed wettability alteration mechanism. No increase in oil recovery observed when injecting brines with high concentrations of SO$_4^{2-}$ ions is also contradictory to the proposed wettability alteration mechanism. Therefore, understanding the fundamental mechanism behind SmW-EOR is quite important. In this study it is attempted to conduct geochemical modeling of salt solubility at reservoir conditions to explore the possible correlation between different brine properties and the corresponding increase in oil recovery (as reported in literature).

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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 CO$_2$ transport applications
In this work the Cubic Plus Association (CPA) equation of state is applied to multicomponent mixtures containing CO$_2$ with alkanes, water, and glycols. Various modelling approaches are used i.e. different association schemes for pure CO$_2$ (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 CO$_2$ with other hydrogen bonding fluids (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). Initially, new binary interaction parameters were estimated for (CO$_2$ + 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 CO$_2$ 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 CO$_2$ with glycols, alcohols and water or alternatively considering CO$_2$ 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.

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Modelling the phase equilibria of multicomponent mixtures containing CO₂, alkanes, water, and/or alcohols using the quadrupolar CPA equation of state

In this work, a quadrupolar cubic plus association (qCPA) equation of state is evaluated for its ability to predict the phase equilibria of multicomponent mixtures containing CO₂ and alkanes, alcohols, and/or water. A single binary interaction parameter is employed in qCPA for all binary combinations. All parameters are based solely on pure fluid or binary mixture
data and multicomponent data are used only to evaluate the predictions. The performance of qCPA is, for all mixtures, compared to CPA where CO₂ is considered to be either non-associating (inert), solvating or self-associating. In the latter two approaches, an additional adjustable parameter is employed for binary pairs of CO₂ and an associating compound. The results show that the predictions with qCPA are very similar to the best performing CPA approaches, even though the model uses fewer adjustable binary parameters. The predictions with qCPA and the best CPA approaches are typically satisfactory and predict the general behaviour of the systems. As expected, qCPA and CPA with solvation or association typically performs better than inert CPA for two- and three phase vapour–liquid and vapour–liquid–liquid equilibria. However, inert CPA yields the best results of all the models for the prediction of dew point pressures.

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- BFI (2008): BFI-level 1
- Scopus rating (2008): SJR 1.003 SNIP 0.765
- Web of Science (2007): Indexed yes
- Scopus rating (2007): SJR 1.088 SNIP 0.775
- Scopus rating (2006): SJR 1.023 SNIP 0.78
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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/recirculation 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 9 mol 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).
Operation and Design of Diabatic Distillation Processes

Diabatic operation of a distillation column implies that heat is exchanged in one or more stages in the column. The most common way of realising diabatic operation is by internal heat integration resulting in a heat-integrated distillation column (HIDiC). When operating the rectifying section at a higher pressure, a driving force for transferring heat from the rectifying section to the stripping section is achieved. As a result, the condenser and reboiler duties can be significantly reduced. For two-product distillation, the HIDiC is a favourable alternative to the conventional distillation column. Energy savings up to 83% are reported for the HIDiC compared to the CDiC, while the reported economical savings are as high as 40%. However, a simpler heat-integrated distillation column configuration exists, which employs compression in order to obtain a direct heat integration between the top vapour and the reboiler. This configuration is called the mechanical vapour recompression column (MVRC). Energy and economic savings of similar magnitude as the HIDiC are reported for the MVRC. Hence, it is important to develop methods and tools for assisting the selection of the best distillation column configuration.

The contributions of this work can be divided in three parts. The first part involves the identification of the preferred distillation column configuration (CDiC, MVRC, or HIDiC) for a given mixture to be separated. Correlations between physical parameters, distillation column design variables, and preliminary feasibility indicators are investigated through simulations studies. The simulation studies include case studies, where different mixtures are separated in different distillation column configurations. The considered mixtures are industrially relevant and their thermodynamic behaviours vary considerably from one another. The HIDiC was found to be the preferred configuration in terms of operating expenditures for mixtures of normal boiling point differences below 10K. The second part involves the investigation of the technological feasibility of the HIDiC. The impact on the column capacity (required tray area, entrainment flooding, weeping) of different column arrangements of the internal heat transfer is investigated. Furthermore, the ability to achieve stable operation of a concentric HIDiC is investigated by systematically designing a regulatory control layer and a supervisory control layer. Stable operation, in terms of column capacity and set point tracking, is demonstrated by simulation. The final part covers the developed simulation tools and methods. A new distillation column model is presented in a generic form such that all the considered distillation column configurations can be described within the same model framework. The following distillation column configurations are considered:

- The conventional distillation column (CDiC)
- The mechanical vapour recompression column (MVRC)
- The heat-integrated distillation column (HIDiC)
- The secondary reflux and vaporisation column (SRVC)

The generic nature of the modelling framework is favourable for benchmarking distillation column configurations. To further facilitate benchmarking of distillation column configurations, a conceptual design algorithm was formulated, which systematically addresses the selection of the design variables. The conceptual design of the heat-integrated distillation column configurations is challenging as a result of the increased number of decision variables compared to the CDiC. Finally, the model is implemented in Matlab and a database of the considered configurations, case studies, pure component properties, and binary interaction parameters is established.

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Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, CERE – Center for Energy Ressources Engineering
Optimizing integrated reference cases in the OCTAVIUS project

Adding a carbon capture plant to a power plant reduces the efficiency of said power plant. In order to keep this drop in efficiency as small as possible, several optimisation studies are performed in the OCTAVIUS project. Based on the work of the European Benchmarking Task Force-EBTF within the CESAR, CAESAR, and DECARBit projects, two reference power plants are modelled in Ebsilon®Professional. The first is an 800 MWe coal case, the second a 430 MWe natural gas combined cycle (NGCC) case. For each power plant two separate capture plants are considered: one using 30 wt% MEA as solvent system, the other with CESAR1, a mixture of AMP and PZ as solvent system. This results in four different reference cases which are optimized by varying different process parameters and evaluating process modifications. In a second step, the integration of the capture plant into the power plant is evaluated. This is important especially for the coal fired power plant, where integration of waste heat from the capture plant or the CO2 compressor intercoolers can lead to a significant increase in overall efficiency. The configuration of intercoolers for the CO2 compressor is adapted to achieve the highest overall efficiency. For the natural gas combined cycle plant, integration is not that beneficial, since there is no heat sink available in the water steam cycle. In the end, the cost of electricity and cost of CO2 avoided is calculated for all four cases. While the CESAR1 solvent system in a conventional absorber-stripper scheme is less costly (almost 17%) than the MEA solvent system in a process with Lean Vapour Compression for the coal cases, the result is the opposite for the two NGCC cases though the difference is not substantial.
New vapor-liquid equilibrium (VLE) data for 1-propanethiol + 1-butanethiol + CH₄ ternary system is reported. Measurements were performed at three different temperatures (303, 336, and 368 K), and the pressure ranged from 1 to 9 MPa. The total system pressure was maintained by CH₄. The inlet mole fraction of 1-propanethiol (x = 5.43 x 10⁻¹) and 1-butanethiol (x = 4.56 x 10⁻¹) in the liquid phase were same in all experiments. A static analytic method was used for performing phase equilibrium measurements. The new VLE data have been modeled successfully with cubic-plus-association (CPA) equation of state.
Phase equilibrium of North Sea oils with polar chemicals: Experiments and CPA modeling

This work consists of a combined experimental and modeling study for oil - MEG - water systems, of relevance to petroleum applications. We present new experimental liquid-liquid equilibrium data for the mutual solubility of two North Sea oils + MEG and North Sea oils + MEG + water systems in the temperature range 303.15-323.15 K and at atmospheric pressure. These new data are for North Sea oils which are substantially heavier and with higher aromatic/naphthenic content compared to previous studies. The new data compare favorably with previously reported measurements for other North Sea oils. The data have been successfully modeled using the Cubic- Plus-Association (CPA) equation of state (EoS) using a previously developed characterization method and new correlations for estimating binary interaction parameters between MEG-hydrocarbons and water-hydrocarbons. The results are in satisfactory agreement to the experimental data, considering especially the complexity of the studied reservoir fluids, in particular their heavy and aromatic character.
Pitfalls of using the geometric-mean combining rule in the density gradient theory

It is popular and attractive to model the interfacial tension using the density gradient theory with the geometric-mean combining rule, in which the same equation of state is used for the interface and bulk phases. The computational efficiency is the most important advantage of this theory. In this work, it has been mathematically shown that the theory fails if the solution profile is not monotonic in the path function, which is defined as the summation of the density multiplied by the square root of the influence parameter over all components. A computational solution procedure is then presented by specifying the path function, in which a reference component is not needed. The differences of the chemical potential between the interface and the bulk phases, and the tangent plane distance have been used to analyze the characteristics of the solution profile from the geometric-mean density gradient theory. It has been found that the solution profile passes a saddle point of the tangent plane distance, which is independent of the influence parameters. It has been shown that the numerical pitfalls could occur for both vapor liquid and liquid liquid equilibrium systems. Shape density change inside the interface could be considered as a warning for the unsuccessful applications of the geometric-mean density gradient theory combined with the chosen thermodynamic model, even if numerical pitfalls do not occur. (C) 2016 Elsevier B.V. All rights reserved.
Prediction and experimental determination of the solubility of exotic scales at high temperatures - Zinc sulfide

The presence of “exotic” scale such as Zinc Sulfide (ZnS), Lead Sulfide (PbS) and Iron Sulfide (FeS) in HP/HT reservoirs has been identified. “Exotic” scale materials come as a new challenge in HP/HT reservoirs. This has led to the development of more advanced tools to predict their behavior at extreme conditions. The aim of this work is to include ZnS into the group of scale materials that can be modeled with the Extended UNIQUAC model. Solubility data for ZnS are scarce in the open literature. In order to improve the available data, we study the experimental behavior of ZnS solubility at high temperatures.

The determination of the solubility of ZnS is carried out at temperatures up to 250°C. Zinc sulfide (99.99%) and ultra-pure water are placed in a vial in a reduced oxygen atmosphere. The sample is placed in a controlled bath and stirred until equilibrium is attained. The suspension is filtered at the same process temperature and diluted immediately. Afterwards the aqueous solution is analyzed using Inductively Coupled Plasma Optical Emission Spectroscopy (ICP-OES) as analytical technique. The concentrations of Zn^{2+} and S^{2-} ions are analyzed. The experimental data are used for parameter estimation in the Extended UNIQUAC model presented by Villafafila et al. (2005); (2006). The solid-liquid phase equilibria of the system is represented using the Extended UNIQUAC model.
model is chosen due to its versatility and fewer number of parameters (two parameters per species plus two parameters per species pair) to be estimated compared to other models (Pitzer's model). It is observed that ZnS solubility increases with increasing the temperature. This temperature dependency is very well represented by the Extended UNIQUAC model. The model is capable of predicting experimental data within the experimental error. The agreement between experimental data and the Extended UNIQUAC model shows that this thermodynamic model is a promising tool capable of determining the occurrence of ZnS scaling in HP/HT reservoirs. This methodology can be extended to other scaling materials (PbS, FeS), making the Extended UNIQUAC model a leading model in predicting scaling in HP/HT reservoirs.

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Predictive screening of ionic liquids for dissolving cellulose and experimental verification
In this work, 357 ionic liquids (ILs) formed from 17 cations and 21 anions were selected for evaluation of their ability to dissolve cellulose by COSMO-RS. In order to evaluate the predictive model and method, experimental measurements of the solubility of microcrystalline cellulose (MCC) in 7 of these ILs were also conducted. Predicted results from logarithmic activity coefficients were generally in good agreement with the experimental results. Three different models were used for describing cellulose, and the mid-monomer part of the cellotriose model was found to be closer to the experimental results than a neat glucose model and the model of the mid-dimer part of cellotetraose. Excess enthalpy calculations indicated that hydrogen-bond (H-bond) interactions between cellulose (i.e. the three cellulose models) and the 7 studied ILs are key factors for the solubility of cellulose, and the anions play a crucial role in the cellulose dissolution process. Importantly, the cations of methylimidazolium+, pyridinium+, ethylmorpholinium+ and methlypyrrolidinium+ structured with functional groups including ethyl, allyl, 2-hydroxyethyl, 2-methoxyethyl and acryloyloxypropyl, combined with anions Ac−, Dec−, HCOO−, Cl−, BEN−, DMPO4−, DEP−, DBP− and Br− were predicted to be the best for dissolving cellulose.

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BFI (2015): BFI-level 2
Probe the Binding Mode of Aristololactam-β-D-glucoside to Phenylalanine Transfer RNA in Silico

Understanding the interactions of drug molecules with biomacromolecules at a micro-scale level is essential to design potent drugs for the treatments of human genome diseases. To unravel the mechanism of binding of aristololactam-β-D-glucoside (ADG) and phenylalanine transfer RNA (tRNA^{Phe}), an integrated computational strategy combining quantum mechanics (QM) calculation, molecular docking and atomistic molecular dynamics (MD) simulation was present in this work. QM calculations were performed to derive the partial charges of ADG, molecular docking was used to determine the binding poses of ADG on the tRNA^{Phe}, and atomistic MD simulations were conducted to examine the thermal stability of five predicted binding poses for the complex of ADG and the tRNA^{Phe}. The binding free energies of the five complexes were then calculated using the molecular mechanics/generalized born surface area approach with the variable internal dielectric constant model. By comparing computed affinities and experimentally-measured values in the binding free energy, we identified a most likely binding structure of ADG and the tRNA^{Phe}. Further analysis of energy of the ADG-tRNA complex revealed that the aristololactam of ADG provides binding specificity to the tRNA^{Phe}, and the D-glucose...
contributes to the affinity for binding with the tRNA^Phe.

**General information**

State: Published  
Organisations: Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering, North Carolina State University, Wuhan Institute of Technology, East China University of Science and Technology  
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**Property Model-based Tailor-made Design of Chemical-based Products**

Computer-aided model-based methods and tools are increasingly playing important roles in chemical product design. They have the potential to very quickly search for and identify reliable product candidates that can then be verified through experiments. In this way, the time and resources spent on experiment are reduced leading to faster and cheaper to market the products. The tools also help to manage the solution of product design problems, which usually require efficient handling of model-data-knowledge from different sources and at different time and size scales.

The main contribution of this project is: (1) the development of a systematic model-based framework for chemical product design; (2) its implementation as a computer-aided tool based on a specially developed architecture; (3) the creation of product design template together with their algorithms, models, tools and data for various types of products. The goal has been to develop a chemical product simulator, similar in concept to a process simulator, which make the product design and development easier and faster, and provide the way for unified and consistent product documentation. In the same way a typical process simulator works, the developed product simulator (VPPD-Lab) allows product designers to: (1) analyze chemicals based products by performing virtual experiments (product property and performance calculations); (2) predict the properties of products; and (3) create new product property and product performance models, when needed. However, unlike process simulators, VPPD-Lab can also be used directly for (4) design of chemicals based products using the design template for various types of products, such as, single molecule products, formulations, blends, emulsions and devices; and, (5) creation of new product design templates when the needed template for a desired product is not available. VPPD-Lab employs a suite of algorithms(such as database search, molecular and mixture blend design) and toolboxes (such as property calculations and property model consistency tests) for specific product property prediction, design, and/or analysis tasks.

In order to achieve the features mentioned above, several issues need to be addressed: the translation of consumer needs into target properties; property models and available data for each type of chemical products; design methods and algorithms; available computer-aided tools; the systematic framework for chemical product design and analysis and its implementation as architecture for VPPD-Lab. From many test problems, eight application examples are presented to illustrate the use of the software. For two of these examples, the prediction of product properties and the use of virtual experiments to test product performances are highlighted. Five examples illustrate the use of the product design templates with respect to five types of chemical products (molecular design, formulation design, emulsion design, blend design and device design).

**General information**

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Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, KT Consortium, CERE – Center for Energy Resources Engineering  
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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.
Solubility Measurements and Modeling of Zinc, Lead and Iron Sulfides at High Temperatures and High Pressures

Solubility measurements of sulfides in aqueous solutions are necessary to understand the behaviour of these scaling minerals in geothermal and oil reservoirs. The low solubility levels of Zinc Sulfide (ZnS), Lead Sulfide (PbS) and Iron Sulfide (FeS) make the solubility measurements a challenging task. Consequently existing data are rare and scattered. The aim of this work is to develop a reliable experimental procedure and to measure solubility of sulfides at high temperature and pressures. Additionally the experimental data are used for estimation of the solid-liquid equilibrium using the Extended UNIQUAC model.

The experimental determination of the solubility of ZnS, PbS and FeS is carried out at temperatures up to 200°C and pressures up to 60 bars. The minerals in their pure form are added to ultra-pure water previously degassed with nitrogen. The aqueous solution is prepared in a reduced oxygen atmosphere to avoid the risk of oxidation of sulfide minerals. The solution is kept in an equilibrium cell at constant temperature and pressure with continuous stirring. The concentration of Zn²⁺, Pb²⁺, Fe²⁺ and S²⁻ are measured using Inductively Coupled Plasma Optical Emission spectrometry (ICP-OES) as analytical technique.

The solid-liquid equilibria is calculated using the Extended UNIQUAC model. The Extended UNIQUAC model is a local composition model and features several advantages compared to other models when describing the behaviour of aqueous electrolytes systems and it was presented by Thomsen and Rasmussen in 1999 1. The model accounts for the dependency of the solubility on pressure and temperature. The pressure parameters were proposed by Villafáfila et al (2005; 2006) 2 on their study on sulfate scaling minerals. The parameter estimation of the model is carried out based on the experimental data produced in our laboratory. The results show that the Extended UNIQUAC model can correlate the solubility data for sulfides within experimental accuracy.

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Authors: Carolina Figueroa Murcia, D. (Intern), Fosbøl, P. L. (Intern), Thomsen, K. (Intern)
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Solubility Modeling of the Binary Systems Fe(NO₃)₃–H₂O, Co(NO₃)₂–H₂O and the Ternary System Fe(NO₃)₃–Co(NO₃)₂–H₂O with the Extended Universal Quasichemical (UNIQUAC) Model

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.
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.

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 Ressources 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
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
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Thermodynamic modeling of CO2 mixtures

Knowledge of the thermodynamic properties and phase equilibria of mixtures containing carbon dioxide (CO2) is important in several industrial processes such as enhanced oil recovery, carbon capture and storage, and supercritical extractions, where CO2 is used as a solvent. Despite this importance, accurate predictions of the thermodynamic properties and phase equilibria of mixtures containing CO2 are challenging with classical models such as the Soave-Redlich-Kwong (SRK) equation of state (EoS). This is believed to be due to the fact that CO2 has a large quadrupole moment which the classical models do not explicitly account for.

In this thesis, in an attempt to obtain a physically more consistent model, the cubic-plus association (CPA) EoS is extended to include quadrupolar interactions. The new quadrupolar CPA (qCPA) can be used with the experimental value of the quadrupole moment and with or without introducing an additional pure compound parameter. In the absence of quadrupolar compounds qCPA reduces to CPA, which itself reduces to SRK in the absence of association. As the number of adjustable parameters in thermodynamic models increase, the parameter estimation problem becomes increasingly complicated due to parameter identifiability issues. In an attempt to quantify and illustrate these issues, the uncertainties in the pure compound parameters of CO2 were investigated using qCPA as well as different CPA approaches. The approaches employ between three and five parameters. The uncertainties in the parameters were propagated to physical properties, vapor liquid equilibria (VLE), and liquid-liquid
equilibria (LLE) using Monte Carlo simulations. The uncertainties in the pure compound parameters were found to be negligible for modeling approaches which employed three adjustable parameters. For modeling approaches with more than three adjustable parameters, however, the uncertainties in the pure compound parameters were significant. As a result, the propagated errors were substantial for certain output properties. The uncertainties in VLE were for instance much larger when qCPA was employed with four parameters rather than three. The uncertainty analysis indicated that the parametrization of multi-parameter models is at least as important as the specific model term.

The new qCPA and several CPA approaches were extensively evaluated for their ability to predict the thermodynamic properties of pure CO2. The predictions of these pure compound properties were satisfactory with qCPA, although similar predictions were achieved with other CPA approaches. The model was subsequently evaluated for its ability to predict and correlate the binary VLE and LLE of mixtures containing CO2 and n-alkanes, water, alcohols, or quadrupolar compounds. For these binary mixtures qCPA appeared to other systematically improved predictions and correlations as compared to the cases where quadrupolar interactions were ignored. The improvements were particularly pronounced for mixtures of CO2 and hydrocarbons where the model is almost fully predictive.

Finally qCPA was evaluated for its ability to predict the phase equilibria of multicomponent mixtures containing CO2 and n-alkanes, water, and/or alcohols. A single binary interaction parameter was employed in qCPA for most binary combinations. Both qCPA and the best CPA approaches typically performed satisfactorily and predicted the general behavior of the systems, but qCPA used fewer adjustable parameters to achieve similar predictions.

It has been demonstrated that qCPA is a promising model which, compared to CPA, systematically improves the predictions of the experimentally determined phase equilibria between binary and ternary mixtures containing CO2 and other non-quadrupolar compounds. However, for mixtures containing two quadrupolar compounds, or quadrupolar and polar compound, considerable uncertainty remains as to whether these mixtures are handled in the best possible way. When binary interaction parameters were employed to correlate experimental phase equilibria data, both qCPA and CPA yielded similar correlations - and predictions in the multicomponent case.

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Thermodynamic modeling of liquid–liquid phase change solvents for CO2 capture
A thermodynamic model based on Extended UNIQUAC framework has been developed in this work for the de-mixing liquid–liquid phase change solvents, DEEA (2-(diethylamino)ethanol) and MAPA (3-(methylamino)propylamine). Parameter estimation was performed for two ternary systems, H2O-DEEA-CO2 and H2O-MAPA-CO2, and a quaternary system, H2O-DEEA-MAPA-CO2 (phase change system), by using different types of experimental data (equilibrium and thermal) consisting of pure amine vapor pressure, vapor-liquid equilibrium, solid-liquid equilibrium, liquid–liquid equilibrium, excess enthalpy, and heat of adsorption of CO2 in aqueous amine solutions. 94 model parameters and 6 thermodynamic properties were fitted to approximately 1500 experimental data. The developed model accurately represents the equilibrium and thermal data for the studied systems with a single unique set of parameters. The model parameters are valid in the temperature range from −25 to 200 °C, CO2 partial pressure from 0 to 945 kPa, and concentration of DEEA, MAPA, and CO2 up to 131, 23, and 33 mol(kg H2O)−1, respectively. The model calculated speciation are also presented for the studied systems. The model developed in this work can be used for process simulation of CO2 capture with aqueous blends of DEEA/MAPA.

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Web of Science (2014): Indexed yes
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Scopus rating (2013): SJR 2.331 SNIP 3.018 CiteScore 5.66
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Scopus rating (2010): SJR 1.481 SNIP 2.436
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Main Research Area: Technical/natural sciences
Uncertainty analysis of the CPA and a quadrupolar CPA equation of state - With emphasis on CO2

The parameters of thermodynamic models, such as the cubic plus association (CPA) equation of state, are subject to uncertainties due to measurement errors in the experimental data that the models are correlated to. More importantly as
the number of adjustable parameters increase, the parameter estimation problem becomes more complicated due to parameter identifiability issues. In this work the uncertainties in the pure compound parameters of CO2 are investigated using several different CPA approaches, including a new quadrupolar CPA. The uncertainties are estimated using both least squares estimation and the bootstrap method for parameter estimation. The uncertainties in the parameters estimated from the bootstrap method are propagated to physical property and vapor liquid equilibrium predictions using Monte Carlo simulations. The results indicate that both the pure compound parameter uncertainty and the propagated uncertainty are negligible for the modeling approaches which employ three adjustable parameters. For modeling approaches with more than three adjustable parameters, however, there may be significant uncertainties in the pure compound parameters, as well as a high degree of correlation between the adjustable parameters. This results in significant propagated errors for certain output properties. To reduce the uncertainty in the adjustable model parameters the heat of vaporization was included as additional correlation data. This resulted in parameter distributions which followed a normal distribution more closely, however, the correlation between the adjustable parameters remained high. Overall the results indicate, that it is important to report parameter uncertainties together with their correlation matrix when a model is developed, so that better informed decisions can be made, for instance about which model extension, or association scheme should be employed.

**General information**

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

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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
- 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
A dynamic mathematical model for packed columns in carbon capture plants

In this paper, we present a dynamic mathematical model for the absorption and desorption columns in a carbon capture plant. Carbon capture plants must be operated in synchronization with the operation of thermal power plants. Dynamic and flexible operation of the carbon capture plant is important as thermal plants must be operated very flexibly to accommodate large shares of intermittent energy sources such as wind and solar in the energy system. To facilitate such operation, dynamic models for simulation, optimization and control system design are crucial. The dynamic model developed in this paper is suitable for gas-liquid packed columns, e.g. for CO2 absorption and desorption. The model is based on rigorous thermodynamic and conservation principles and it is set up to preserve these properties upon numerical integration in time. The developed model is applied for CO2 absorption and desorption simulation using monoethanolamine (MEA) and piperazine (PZ) as solvent. MEA is considered as the base-case solvent in the carbon capture business. The effect of changes in the flue gas flow rate and changes in the available steam are investigated to determine their influence on the performance of the capture process. The response of the model is shown in terms of capture efficiency and purity of the CO2 product stream. The model is aimed for rigorous dynamic simulation in the context of optimization and control strategy development.

General information
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Organisations: Department of Chemical and Biochemical Engineering, CERE – Center for Energy Ressources Engineering, Department of Applied Mathematics and Computer Science , Scientific Computing
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Main Research Area: Technical/natural sciences
A general enhancement factor model for absorption and desorption systems: A CO$_2$ 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 CO$_2$-MEA-H$_2$O 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 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 Resources Engineering
Authors: Gaspar, J. (Intern), Fosbøl, P. L. (Intern)
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BFI (2017): BFI-level 2
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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
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.
BFI (2017): BFI-level 2
Web of Science (2017): Indexed Yes
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Scopus rating (2016): CiteScore 3.11 SJR 1.034 SNIP 1.268
Web of Science (2016): Indexed yes
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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
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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 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
Scopus rating (2011): SJR 1.004 SNIP 1.234 CiteScore 2.31
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
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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
Scopus rating (2007): SJR 1.256 SNIP 1.341
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
Web of Science (2005): Indexed yes
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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Source-ID: 275641169
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 has been less explored. In this study the relative affinity between different ions and the oil surface 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

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: Chakravarty, K. H. (Intern), Fosbøl, P. L. (Intern), Thomsen, K. (Intern)
Pages: 817-836
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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.

General information
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Organisations: Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering, IFP Energies nouvelles
Authors: Nguyen, T. (Ekstern), de Hemptinne, J. (Ekstern), Creton, B. (Ekstern), Kontogeorgis, G. M. (Intern)
Pages: 7230−7241
Control of a post-combustion CO2 capture plant during process start-up and load variations
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. [All rights reserved Elsevier].
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 cm^3·mol^-1 for the n-hexane + n-decane system and 7.65 cm^3·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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Organisations: Department of Chemistry, CERE – Center for Energy Ressources Engineering, Center for Energy Resources Engineering
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Publication information
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
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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
Web of Science (2015): Indexed yes
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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
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/m³) 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 KHi's 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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Organisations: Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering, CHEC Research Centre
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Pages: 554-560
Publication date: 2015
Main Research Area: Technical/natural sciences
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. Most students were involved in cardiology (14.1%). 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. 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.

General information
State: Published
Organisations: Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering, University of Copenhagen, Rigshospitalet
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BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 0.92 SJR 0.415 SNIP 0.528
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.325 SNIP 0.393 CiteScore 0.78
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
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BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.254 SNIP 0.404 CiteScore 0.54
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BFI (2012): BFI-level 1
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ISI indexed (2012): ISI indexed no
BFI (2011): BFI-level 1
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ISI indexed (2011): ISI indexed no
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.402 SNIP 0.672
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.

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Formation of Anhydrite due to Interaction Between Water Soluble CO_2 (aq) and Calcite Mineral During Enhanced Oil Recovery
In the Low Salinity based EOR method, formation and migration of fines have proved to have profound effect on the displacement efficiency of residual oil. Salinity variations of injected brines have also been shown to affect oil recovery for WAG-CO_2 processes. But the effect of fines in EOR during LSWAG-CO_2 has not been previously studied. This study explores the possibility of fines formation during CO_2 injection and attempts to understand its implication in EOR. In this study we use the Extended UNIQUAC model to calculate the possibility of fines formation during CO_2 injection. Detailed simulations were conducted over a temperature range of 50°C to 250°C and a pressure range of 5 bars to 500 bars. The amounts of fines formation taking place for different LSWAG-CO_2 processes were correlated to the described oil recovery. It is observed that significant amounts of fines formation can take place during CO_2 injection in limestone reservoirs. At reservoir conditions, a considerable fraction of the injected CO_2 becomes soluble in sea water. This dissolved CO_2 causes dissolution of CaCO_3 from the mineral surface and releases Ca^{2+} ions into the pore space. Excess Ca^{2+} ions form anhydrite fines with the available SO_4^{2-} ions. The salinity and composition of brines present in pore space shows direct correlation with the amount of fines produced during CO_2 injection. With increase in temperature and pressure, the amount fines formation increased significantly. The described oil recovery for different LSWAG injections showed a consistent correlation with the amounts of fines formation taking place in the pore space. The amount of mineral
dissolution taking place was also precisely calculated using the Extended UNIQUAC model. Good correlation was also observed between calculated amounts of mineral dissolution and the observed increase in permeability. Copyright: 2015 Society of Petroleum Engineers

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**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.

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Organisations: Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering, CERE – Center for Energy Resources Engineering
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**Influence of different SSF conditions on ethanol production from corn stover at high solids loadings**
In this study, three different kinds of simultaneous saccharification and fermentation (SSF) of washed pretreated corn stover with water-insoluble solids (WIS) content of 20% were investigated to find which one resulted in highest ethanol yield at high-solids loadings. The different methods were batch SSF, prehydrolysis followed by batch SSF and fed-batch 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.
Interactions of fines with base fractions of oil and its implication in smart water flooding

Migration of fines, and formation of oil emulsion have been independently observed during smart water flooding both have been suggested to play a vital role in enhanced oil recovery (EOR). But, the exact role of fines and the reason of emulsion formation are not well studied for carbonate reservoirs. This study shows that addition of water and crude oil on calcite fines leads to formation of soluble oil emulsions in the water phase. Formation of these emulsions and its implication in EOR has been experimentally analyzed.

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.
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 equilibrium data measured. A good agreement between predictions and experimental data is observed, supporting the reliability of the new data. (C) 2015 Elsevier B.V. All rights reserved.
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.
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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Modeling of Salinity Effects on Waterflooding of Petroleum Reservoirs

Smart Water flooding is an enhanced oil recovery (EOR) technique that is based on the injection of chemistry-optimized water with changed ionic composition and salinity into petroleum reservoirs. Extensive research that has been carried out over the past two decades has clearly demonstrated that smart water flooding can improve the ultimate oil recovery both in carbonate and sandstone reservoirs. A number of different physicochemical mechanisms of action were proposed to explain the smart water effects, but none of them has commonly been accepted as a determining mechanism.

Most of the experimental studies concerning the smart water effects recognize importance of the chemistry of reservoir rocks that manifests itself in dissolution and precipitation of rock minerals and adsorption of specific ions on the rock surface. The brine-rock interactions may affect the wetting state of the rock and in some cases result in mobilization of the trapped oil.

In this thesis, we set up a generic model for the reactive transport in porous media to investigate how different mechanisms influence the oil recovery, pressure distribution and composition of the brine during forced displacement. We consider several phenomena related to the smart water effects, such as mineral dissolution, adsorption of potential determining ions in carbonate rocks, and mechanisms that influence mobilization of the trapped oil and its transport. Dissolution of minerals occurs due to the different compositions of the injected brine and the formation water that is initially in equilibrium with the reservoir rock. We consider a displacement process in one dimension with dissolution affecting both the porosity/permeability of the rock and the density of the brine. Extending previous studies, we account for the different individual volumes of mineral in solid and in solution, which is found to affect slightly the velocity of the displacement front. The rate of dissolution is found to have a significant influence on the evolution of the rock properties. At low reaction rates, dissolution occurs across the entire region between the injection and production sites resulting in heterogeneous porosity and permeability fields. Fast dissolution resembles formation of wormholes with a significant change in porosity and permeability close to the injection site.

Further, we study the mechanisms that can govern the mobilization of residual oil and its flow in porous media. The oil trapped in the swept zones after conventional flooding is present in a form of disconnected oil drops, or oil ganglia. While the macroscopic theory of multiphase flow assumes that fluid phases flow in their own pore networks and do not influence
each other, the flow of disconnected oil ganglia requires an alternative description. We address this problem by considering a micromodel for the two-phase flow in a single angular pore-body.

On the micro-level, both fluids can be present in a single pore body and interact during the flow. Considering water-wet systems, we find that presence of the water on the surface of the rock and in the corner filaments of pore bodies results in a larger velocity of the viscous flow of the oil phase due to the increased area of the moving oil-water interface. Moreover, the flow of oil may be induced solely by the action of viscous forces at the oil-water interface, which appears to be a new mechanism for the transport of disconnected oil ganglia in porous media. We derive correlations that allow calculating the flow velocities of fluid phases in single pore bodies based on the pore fluid saturations. Based on the microscale considerations, we develop a macroscopic model of displacement accounting for the effects associated with oil ganglia.

The model is based on the assumption that wettability alteration toward increased water-wetness caused by the presence of active species in the injected brine results in formation of the wetting films on the surface of the rock. Oil ganglia are mobilized and carried by the slow flow of wetting films. Considering simplistic pore-network model, we derive the macroscopic system of equations involving description of the transport of oil ganglia. As a result of numerical modeling of the tertiary recovery process, it is found that production of oil ganglia may continue for a long time of injection of around 10 to 20 PVI.

Unlike the conventional models of chemical flooding, where mobilized oil bank travels ahead of the concentration front, the oil ganglia model predicts that the mobilized oil is produced after the active species reaches the effluent. Further extension of the model is achieved by introduction of the non-equilibrium alteration of wettability and non-instantaneous oil mobilization. Such modifications may explain the delay observed in some experiments, where mobilized oil is produced during a long time after several pore volumes of injection.

One of the possible chemical mechanisms through which the mobilization of the residual oil may occur in carbonates is alteration of the electrostatic potential of the surface. Reduction of the surface charge due to adsorption of the potential determining ions results in the decrease in oil affinity towards the surface of the rock. We establish a mathematical model that takes into account adsorption of the potential determining ions: calcium, magnesium, and sulfate, on the chalk surface, to investigate how the composition of the injected brine affects the equilibrium surface composition and how adsorption process affects the composition of the produced brine. We use experimental data on the produced brine composition from the flow-through experiments to estimate the parameters of the adsorption model. The computations suggest that there is no evidence of usually assumed stronger adsorption of magnesium ion compared to calcium at high temperatures. In order to investigate the effect of surface composition on the flooding efficiency, we combine the adsorption model with the Buckley-Leverett model and perform simulations of the experiments concerning flooding in the carbonates.

Computations of the equilibrium surface composition demonstrate a correlation between the concentration of the adsorbed sulfate and the ultimate recovery observed in the experiments indicating that a more negatively charged surface of chalk could be a factor that affects the recovery efficiency without wettability modification.

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Modeling phase equilibria for acid gas mixtures using the CPA equation of state. Part IV. Applications to mixtures of CO2 with alkanes
The thermodynamic properties of pure gaseous, liquid or supercritical CO2 and CO2 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 CO2-alkane mixtures. CPA calculations were performed using different association schemes for
CO₂. Firstly, CO₂ was treated as non-associating fluid and, at a second level, CO₂ 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 CO₂-alkane mixtures has been performed. Mixtures with alkanes up to n-hexatriacontane (n-C₃₆) were investigated and the corresponding binary interaction parameters were estimated with all modeling approaches for CO₂. CPA parameters were previously available for alkanes up to n-eicosane (n-C₂₀) 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.
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.

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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 and petroleum fluid + MEG + 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...
Modeling Water Saturation Points in Natural Gas Streams Containing \( \text{CO}_2 \) and \( \text{H}_2\text{S} \)-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, \( \text{CO}_2 \), and sometimes \( \text{H}_2\text{S} \). 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 at 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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BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.055 SNIP 1.483 CiteScore 3.03
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BFI (2010): BFI-level 1
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Monte Carlo reservoir analysis combining seismic reflection data and informed priors

Determination of a petroleum reservoir structure and rock bulk properties relies extensively on inference from reflection seismology. However, classic deterministic methods to invert seismic data for reservoir properties suffer from some limitations, among which are the difficulty of handling complex, possibly nonlinear forward models, and the lack of robust uncertainty estimations. To overcome these limitations, we studied a methodology to invert seismic reflection data in the framework of the probabilistic approach to inverse problems, using a Markov chain Monte Carlo (McMC) algorithm with the goal to directly infer the rock facies and porosity of a target reservoir zone. We thus combined a rock-physics model with seismic data in a single inversion algorithm. For large data sets, the McMC method may become computationally impractical, so we relied on multiple-point-based a priori information to quantify geologically plausible models. We tested this methodology on a synthetic reservoir model. The solution of the inverse problem was then represented by a collection of facies and porosity reservoir models, which were samples of the posterior distribution. The final product included probability maps of the reservoir properties in obtained by performing statistical analysis on the collection of solutions.

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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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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.

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Scopus rating (2014): SJR 1.012 SNIP 1.292 CiteScore 2.85
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BFI (2013): BFI-level 2
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Web of Science (2011): Indexed yes
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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.

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Scopus rating (2014): SJR 1.667 SNIP 2.331 CiteScore 4.14
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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
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%.

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Organisations: Center for Energy Resources Engineering, Department of Chemistry, Department of Chemical and Biochemical Engineering, CERÉ - Center for Energy Resources Engineering, University of Santiago de Compostela, University of Valladolid, Universidad de Santiago de Compostela
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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.

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.

**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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**Pressure dependence of the solubility of light fullerenes in 1-hexanol from 298.15 K to 363.15 K**

The solubility of light fullerenes (C60 and C70) 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 C60-1-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 C60 and non-solvated C60). The composition of the solid crystallosolvate was determined by thermogravimetric analysis. The solubility diagram of the binary system C70-1-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 C70.

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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 Anaerobaculum, Petrotoga, and Methanothermococcus were enriched. Addition of nitrate favored the growth of Petrotoga over Anaerobaculum. The microbial growth caused changes in the crude oil–brine system: formation of oil emulsions, and reduction in 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.

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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, Teknologisk Institut
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.
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.

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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 Resources Engineering
Authors: Katika, K. (Intern), Halim, A. Y. (Intern), Shapiro, A. (Intern), Fabricius, I. L. (Intern)
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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.

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.
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ISI indexed (2013): ISI indexed yes
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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, carboxydrases, 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.

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Organisations: Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering, CAPEC-PROCESS, Technical University of Denmark, Novozymes A/S
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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.
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.
Thermodynamic modeling of CO₂ 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 CO₂-MDEA-H₂O system are presented. Different types of experimental data consisting of pure MDEA vapor pressure, vapor-liquid equilibrium (VLE) (total pressure and CO₂ 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 CO₂ partial pressure of 0-6161.5 kPa.

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Organisations: Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering, CERE – Center for Energy Resources Engineering, Department of Chemistry
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Scopus rating (2014): SJR 1.667 SNIP 2.331 CiteScore 4.14
Web of Science (2014): Indexed yes
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Scopus rating (2013): SJR 1.811 SNIP 2.595 CiteScore 4.31
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.

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Authors: Sadegh, N. (Intern), Stenby, E. H. (Intern), Thomsen, K. (Intern)
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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.


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.
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, house-hold 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.
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.
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 qC. 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 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.
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 experimental techniques, therefore a systematic approach, integrating model-based as well as experiment-based techniques, for design of these products could significantly reduce both time and cost connected to product development by doing only the necessary experiments, and ensuring chances for innovation. The main contribution of this project is 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 problem definition stage, the consumer needs are translated into a set of target thermo-physical properties and into a list of categories of ingredients that are to be included in the formulation. In the model-based design stage, structured databases...
dedicated algorithms and a property model library are employed for designing 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 experiments. The formulation is then validated or, if necessary, reefined thanks to a systematic list of action. The problem definition stage relies on a robust knowledge base, which needs to systemically generate quantitative, useful input information for the model-based stage, starting from the consumer assessments. In the model-based stage, comprehensive chemical databases, consistent property models and a dedicated algorithm for the design of emulsified solvent mixtures are needed. Finally, for the experiment-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, systematic knowledge base has been developed in relation to emulsified formulated products; chemical 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 been implemented 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 applied, while for the other two, only the first two stages and part of the experiment-based verification 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.
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.

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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.

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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.
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.

**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**

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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.

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Development of an Electrolyte CPA Equation of state for Applications in the Petroleum and Chemical Industries

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 fasion, 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 resuing 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.

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**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.

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Enzymatically Assisted CO₂ Removal from Flue-Gas

The enzyme carbonic anhydrase is an enzyme known to enhance CO₂ 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 show 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.

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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.

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Copyright: 2013 Published by Elsevier Ltd. This is an open access article under the CC BY-NC-ND license (http://creativecommons.org/licenses/by-nc-nd/3.0/).
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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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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From abstract to peer-reviewed publication: country matters

Medical conferences are key in the sharing of new scientific findings. However, results reported as conference-abstracts are generally not considered final before publication in a peer-reviewed journal. It is known that approximately 1/3 of the scientific results presented as abstracts at large medical conferences are published within 2 years of presentation [1] and [2]. Cardiovascular research has increased substantially in the last decade, and low- and middle-income countries have now a greater share of citations than before [3]. Less is known about the relative difference between countries in regard to likelihood of publication and a comparison of abstract-to-publication conversion rate between countries is of interest [4]. By identifying and quantifying country differences, the scientific community could identify barriers for publication and publication bias.

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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.

Impact of soil amendments and the plant rhizosphere on PAH behaviour in soil

Carbonaceous amendments reduce PAH dissolved concentrations ($C_{\text{free}}$), limiting their uptake and toxicity. A soil contaminated with PAHs was mixed with activated carbon (AC), charcoal or compost and planted with radish (Raphanus sativus L.), and $C_{\text{free}}$ and diffusive uptake of the PAHs measured over 2 months. For AC, $C_{\text{free}}$ and diffusive uptake were decreased by up to 94% compared to the unamended soil within one week. In addition, the sum chemical activity of the PAHs remained below the threshold for baseline toxicity. In contrast, charcoal and compost only led to modest reductions in $C_{\text{free}}$ and diffusive uptake, with sum chemical activities that could potentially result in baseline toxicity being observed. Furthermore, both $C_{\text{free}}$ and diffusive uptake were lower in the planted compared to unplanted soils. Therefore, only AC successfully reduced PAH acute toxicity in the soil, but plant-promoted microbial degradation may also play an important role in PAH attenuation.
Radish (Raphanus sativus L.), Freely dissolved concentration, Chemical activity, Diffusive uptake, Passive sampling

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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/butyrate, n-aliphatic acids), it is proposed to consider cross-association in addition to a binary interaction parameter lij on the combining rules for the cross-segment diameter between water and the investigated compound. The binary interaction parameters lij, uαβ, and wαβ 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.
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.

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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 $k_{ij}$ between the components present in the system, is usually enough to describe the solubility of all phases. Accurate predictions are made for VLLE of an aqueous 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 $k_{ij}$ for all MEG-HC pairs. Similarly, the mutual solubility of condensate/oil, MEG and water is predicted satisfactorily using correlations for $k_{ij}$ 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.

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.
Modelling 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.
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.

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ISI indexed (2011): ISI indexed yes
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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. 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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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.

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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 tielines for constant K-values.

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- Scopus rating (2012): SJR 1.066 SNIP 1.338 CiteScore 2.56
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- BFI (2010): BFI-level 2
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- 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
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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- Scopus rating (2015): SJR 0.874 SNIP 0.998 CiteScore 1.99
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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
- 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
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.
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.

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Scopus rating (2014): SJR 0.663 SNIP 0.915 CiteScore 1.84
Web of Science (2014): Indexed yes
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Scopus rating (2013): SJR 0.634 SNIP 1.104 CiteScore 1.98
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BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.523 SNIP 1.255 CiteScore 1.67
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Scopus rating (2010): SJR 0.516 SNIP 0.717
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Scopus rating (2009): SJR 0.654 SNIP 0.815
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Scopus rating (2008): SJR 0.541 SNIP 0.809
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Scopus rating (2005): SJR 0.446 SNIP 0.523
Scopus rating (2004): SJR 0.338 SNIP 0.356
Scopus rating (2003): SJR 0.233 SNIP 0.419
Scopus rating (2002): SJR 0.252 SNIP 0.221
Scopus rating (2001): SJR 0.428 SNIP 0.568
Scopus rating (2000): SJR 0.197 SNIP 0.17
Scopus rating (1999): SJR 0.496 SNIP 0.519
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.
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.

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
Authors: Nielsen, S. M. (Intern), Nesterov, I. (Intern), Shapiro, A. (Intern)
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

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Scopus rating (2011): SJR 0.918 SNIP 1.505 CiteScore 2.42
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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.
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 PCSAFT EOS on liquid-liquid equilibria of water with hydrocarbons has been under debate for some vii 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.

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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.

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Engineering, CHERC Research Centre, Center for Energy Resources Engineering
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Web of Science (2009): Indexed yes
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Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 1.193 SNIP 1.301
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The Virtual Product-Process Design Lab

General information
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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.

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.
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-MDEA-MEA-H₂O, H₂S-MDEA-PZ-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-CH₄-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.
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.
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 steam 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 33m^3/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 4.2L/min and below. The results showed that it was possible to achieve 80% recovery with 3.3m 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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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 approaches 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.
Fluid phase behaviour, Aqueous, Tetrahydrofuran, Modelling, Cubic-plus-association (CPA), Thermodynamics

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**Association models for petroleum applications**

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, asphaltenes, 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 ($F_{AT}$), 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 rc, 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.

**General information**

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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.
BINARY VLE of DEEA/H2O, MAPA/H2O and DEEA/MAPA SYSTEMS

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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
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.
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.

General information

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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.

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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.

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Emulsions, Formulations, Product Design, Property Models, Hand-wash
**Design of an Emulsion-based Personal Detergent through a Model-based Chemical Product Design Methodology**

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**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 experimental stage for final selection and product development is applied. In this way, the whole design procedure speeds up, saving time and money, and the optimum formulation is identified, since a broad range of alternatives are investigated. The approach adopted for the design of emulsion-based chemical products consists in a systematic model-based methodology employing seven hierarchical steps: starting with the identification of the product needs and their translation into appropriate target properties, then building the formulation by adding, one-by-one, the different classes of chemicals needed for each function: from the active ingredients, to the solvents, the emulsifiers and the additives, and finally determining the optimal composition of the formulated product. The design of the ingredients, driven by selection criteria based on the functional properties of each category of chemicals as well as by consideration of effectiveness, safety, toxicity and cost, is done through a data-model based computer aided molecular design technique. When a model-based design is not applicable since the functional properties needed to perform a rigorous choice are not readily available for consideration in a product design methodology, rule-based selection criteria are applied. These are centered on structured databases, where some relevant properties (e.g. safety or toxicity-related), if not available, are predicted through dedicated pure component property models. Once all the most advantageous ingredients have been chosen, the recipe candidates are identified through a knowledge-based mixture design method, where economic considerations are included together with appropriate boundaries related to solubility, stability, toxicity and safety issues. A special database of chemicals, classified according to their function and associated properties, has been developed. Also, a model library consisting of pure component and mixture property models has been developed so that the needed functional properties can be reliably predicted when their data cannot be found in the database. The abovementioned methodology and related tools are generic, in the sense that many different emulsified products can be designed through this framework once the needs-property relations are established, and they are here highlighted through a case-study dealing with the design of a tank cleaning blend. The main focus of this contribution is on the design of surfactants, primary responsible for the cleaning activity, thanks to a comprehensive framework based on newly developed both pure component and mixture property models. The workflow methodology with associated models, tools, databases and algorithms will be implemented into a computer-aided framework for emulsion-based formulation design.

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Development and Analysis of Group Contribution Plus Models for Property Prediction of Organic Chemical Systems

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-ContributionPlus (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 development.

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 sulfurred 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.

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Development of a general model for determination of thermal conductivity of liquid chemical compounds at atmospheric pressure

In this communication, a general model for representation/presentation of the liquid thermal conductivity of chemical compounds (mostly organic) at 1 atm pressure for temperatures below normal boiling point and at saturation pressure for temperatures above the normal boiling point is developed using the Gene Expression Programming algorithm. Approximately 19,000 liquid thermal conductivity data at different temperatures related to 1636 chemical compounds collected from the DIPPR 801 database are used to obtain the model as well as to assess its predictive capability. The parameters of the model comprise temperature, acentric factor, critical pressure, normal boiling temperature, and molecular weight. Nearly 80% of the data set (15,221 data) is randomly assigned to develop the model equation, 10% of the data set (1902 data) is used to validate the model, and the remaining data (1902 data) were implemented to evaluate its predictive power. The average absolute relative deviation of the model results from the DIPPR 801 data is less than 9%. In terms of simplicity and wide range of applicability, this empirical model shows acceptable accuracy. © 2012 American Institute of Chemical Engineers AIChE J, 59: 1702–1708, 2013
Development of a New Comprehensive Framework for Surfactant Selection and Design for Emulsion-based Chemical Product Design

General information
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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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Main Research Area: Technical/natural sciences
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Source-ID: u::9017
Publication: Research - peer-review › Poster – Annual report year: 2013

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

**General information**

- **State:** Published
- **Organisations:** Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering, Islamic Azad University, MINES ParisTech, Saman Energy Giti Co.
- **Authors:** Gharagheizi, F. (Ekstern), Eslamimanesh, A. (Ekstern), Sattari, M. (Ekstern), Mohammadi, A. H. (Ekstern), Richon, D. (Intern)
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  - 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
  - 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
  - Scopus rating (2007): SJR 1.256 SNIP 1.341
  - Web of Science (2007): Indexed yes
  - Scopus rating (2006): SJR 1.483 SNIP 1.612
  - Web of Science (2006): Indexed yes
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 + 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 the vapor phase compositions partially due to uncertainties in the experimental data. © 2012 Elsevier B.V.
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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
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Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 0.966 SNIP 1.284
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Equilibrium Solubility of CO2 in Alkanolamines

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Source-ID: u::7662
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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-alcohols. 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-alcohols, 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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Organisations: Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering, University of Stellenbosch
Authors: de Villiers, A. (Ekstern), Schwarz, C. (Ekstern), Burger, A. (Ekstern), Kontogeorgis, G. (Intern)
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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
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
Authors: Tsivintzelis, I. (Intern), Musko, N. E. (Intern), Baiker, A. (Ekstern), Grunwaldt, J. (Intern), Kontogeorgis, G. (Intern)
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BFI (2017): BFI-level 2
Web of Science (2017): Indexed Yes
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Scopus rating (2016): CiteScore 3.01 SJR 0.976 SNIP 1.266
Web of Science (2016): Indexed yes
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
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Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
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Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.055 SNIP 1.483 CiteScore 3.03
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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
Scopus rating (2007): SJR 1.197 SNIP 1.576
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 0.902 SNIP 1.383
Scopus rating (2005): SJR 1.412 SNIP 1.612
Scopus rating (2004): SJR 1.065 SNIP 1.531
Scopus rating (2003): SJR 1.235 SNIP 1.34
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 1.124 SNIP 1.321
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.
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.
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.

General information
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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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Web of Science (2016): Indexed yes
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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Publication: Research - peer-review › Conference article – Annual report year: 2013
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.

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Web of Science (2017): Indexed Yes
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Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
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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
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
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-cyclicguanidinium 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.
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.
Liquid–liquid equilibria for reservoir fluids + monoethylene glycol and reservoir fluids + monoethylene glycol + water: Experimental measurements and modeling using the CPA EoS

The complex phase equilibrium between reservoir fluids and associating compounds like water and glycols has become more and more 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. This work presents new phase equilibrium data for binary MEG/reservoir fluid and ternary MEG/water/reservoir fluid systems, where two reservoir fluids from Statoil operated fields are used. The solubility data are reported over a range of temperatures and compositions at atmospheric pressure. The CPA equation of state has been applied to systems containing reservoir fluids, MEG and water. With a minimum number of adjustable parameters from binary pairs, the CPA EoS satisfactorily describes the mutual solubility of the binary systems reservoir fluid and MEG. Promising results are also obtained with CPA EoS for ternary mixtures, with some deviations for the solubility of MEG/water in the hydrocarbon phase and for the hydrocarbons in the polar phase.

General information
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BFI (2009): BFI-level 2
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Web of Science (2009): Indexed yes
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Scopus rating (2008): SJR 1.227 SNIP 1.09
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.
Modeling of the Critical Micelle Concentration (CMC) of Nonionic Surfactants with an Extended Group- Contribution Method

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.

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Main Research Area: Technical/natural sciences
Molasses injection as a MEOR strategy: Enrichment incubations of brine/oil from North Sea Oil Field

General information
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Main Research Area: Technical/natural sciences

Numerical analysis of a one-dimensional multicomponent 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.

General information
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Web of Science (2015): Indexed yes
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.

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Organisations: Department of Micro- and Nanotechnology, Nanoprobes, Department of Chemistry, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering, Center for Energy Resources Engineering
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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 are employed, but improvements can in some cases be as large as 45%. 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.
Predicting 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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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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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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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 peer-reviewed full manuscript publications of these abstracts. 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.

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Scopus rating (2011): SJR 0.718 SNIP 0.746 CiteScore 1.39
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Scopus rating (2010): SJR 0.538 SNIP 0.5
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.616 SNIP 0.594
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Scopus rating (2008): SJR 0.614 SNIP 0.566
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Scopus rating (2005): SJR 0.69 SNIP 0.703
Scopus rating (2004): SJR 0.526 SNIP 0.654
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Organisations: Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering, Duke University
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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 approach 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 multinominal 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. The proposed methodology allows us to invert seismic reflection data for rock properties, namely for porosity, by integrating rock physics model into inversion procedure. Errors associated with conversion from depth to time are handled with a novel mapping approach. 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.

General information
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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.

General information
State: Published
Organisations: Center for Energy Resources Engineering, CERE – Center for Energy Resources Engineering, Department of Chemistry, Department of Chemical and Biochemical Engineering, Eni, University of Bergen
Study of Crystallization Kinetics Within a Generic Modelling Framework

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Process Engineering and Technology, Center for Energy Resources Engineering, CERE – Center for Energy Resources Engineering, Loughborough University
Publication date: 2013
Main Research Area: Technical/natural sciences
Source: dtu
Source-ID: u::9431
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2013

Study on the Application of the Tie-Line-Table-Look-Up-Based Methods to Flash Calculations in Compositional Simulations

Flash calculation can be a time-consuming part in compositional reservoir simulations, and several approaches have been proposed to speed it up. One recent approach is the shadow-region method that reduces the computation time mainly by skipping stability analysis for a large portion of the compositions in the single-phase region. In the two-phase region, a highly efficient Newton-Raphson algorithm can be used with the initial estimates from the previous step. Another approach is the compositional-space adaptive-tabulation (CSAT) approach, which is based on tie-line table look-up (TTL). It saves computation time by replacing rigorous phase-equilibrium calculations with the stored results in a tie-line table whenever the new feed composition is on one of the stored tie-lines within a certain tolerance. In this study, a modified version of CSAT, named the TTL method, has been proposed to investigate if approximation by looking up a tie-line table can save flash-computation time in the two-phase region. The number of tie-lines stored for comparison and the tolerance set for accepting the feed composition are the key parameters in this method because they will influence the simulation speed and the accuracy of simulation results. We also proposed the tie-line distance-based approximation (TDBA) method, an alternative method to TTL, to obtain approximate flash results in the two-phase region. The method uses the distance to a 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
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Pages: 932-942
Publication date: 2013
Main Research Area: Technical/natural sciences

Publication information
Journal: S P E Journal
Volume: 18
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.

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: Daraboina, N. (Intern), Malmos, C. (Intern), von Solms, N. (Intern)
Pages: 749-757
Publication date: 2013
Main Research Area: Technical/natural sciences
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
State: Published
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
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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.
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: Karakatsani, E. K. (Intern), Kontogeorgis, G. M. (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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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
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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
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BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.047 SNIP 1.165
Web of Science (2010): Indexed yes
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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
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
Thermodynamic promotion of carbon dioxide-clathrate hydrate formation by tetrahydrofuran, cyclopentane and their mixtures

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 283.3 K to 285.2 K. At 283.3 K, the three-phase equilibrium pressure is determined to be 0.61 MPa (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 285.2 K down to 275.5 K. 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 275.1 K to 286.6 K. 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

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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Number of pages: 27
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Main Research Area: Technical/natural sciences
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CCSConference2013_Antwerp_Final.pdf

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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, Computer Aided Process Engineering Center, CERE – Center for Energy Ressources Engineering
Authors: Mattei, M. (Intern), Kontogeorgis, G. (Intern), Gani, R. (Intern)
Number of pages: 2
Publication date: 2013
Main Research Area: Technical/natural sciences

Bibliographical note
Oral presentation
Vapor-Liquid Equilibrium of CO2 with Aqueous Solutions of DEEA, MAPA and their Mixture

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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
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Vapor-liquid equilibrium, Post-combustion capture, Calorimeter, Phase change solvents, Amine, N,N-diethylethanolamine (DEEA), 3-Methylamino propylamine (MAPA)
Electronic versions:
PCCC2-Abstract_Mwa.pdf

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Source-ID: u::8737
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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-butanol + 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

General information
State: Published
Organisations: Center for Energy Resources Engineering, CERE – Center for Energy Ressources Engineering, Department of Chemical and Biochemical Engineering, MINES ParisTech
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Pages: 2014698-14705
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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
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 Ressources Engineering, University of Lorraine, IFP Energies nouvelles
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.

General information
State: Published
Organisations: Center for Energy Resources Engineering, Department of Chemistry, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering
Authors: Michelsen, M. L. (Intern), Yan, W. (Intern), Stenby, E. H. (Intern)
Number of pages: 11
Publication date: 2012
Main Research Area: Technical/natural sciences
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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 solution 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
State: Published
Organisations: Center for Energy Resources Engineering, Department of Informatics and Mathematical Modeling, Scientific Computing, CERE – Center for Energy Resources Engineering
Authors: Lange, K. (Intern), Frydendall, J. (Intern), Cordua, K. S. (Intern), Hansen, T. M. (Intern), Melnikova, Y. (Intern), Mosegaard, K. (Intern)
Pages: 783-803
Publication date: 2012
Main Research Area: Technical/natural sciences

Publication Information
Journal: Mathematical Geosciences
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Ratings:
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.

**General information**
State: Published
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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Number of pages: 21
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Main Research Area: Technical/natural sciences
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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**
State: Published
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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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
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–Smolukowski 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
Application of the UNIFAC-CI Model for Phase Equilibria Predictions of Organic Chemical System

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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Scopus rating (2014): SJR 1.012 SNIP 1.292 CiteScore 2.85
Web of Science (2014): Indexed yes
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ISI indexed (2013): ISI indexed yes
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Scopus rating (2012): SJR 1.066 SNIP 1.338 CiteScore 2.56
ISI indexed (2012): ISI indexed yes
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Scopus rating (2011): SJR 1.086 SNIP 1.24 CiteScore 2.58
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BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.002 SNIP 1.164
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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
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Original language: English
Speed of sound, EOS, PC-SAFT, Universal constants, Parameter estimation
Electronic versions:
A statistical method for evaluation of the experimental phase equilibrium data of simple clathrate hydrates

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.

General information
State: Published
Organisations: Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering, MINES ParisTech, Islamic Azad University
Authors: Eslamimanesh, A. (Ekstern), Gharagheizi, F. (Ekstern), Mohammadi, A. H. (Ekstern), Richon, D. (Intern)
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Main Research Area: Technical/natural sciences

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Scopus rating (2016): CiteScore 3.05 SJR 1.037 SNIP 1.442
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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
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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
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.

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
Authors: Mattei, M. (Intern), Kontogeorgis, G. (Intern), Gani, R. (Intern)
A Systematic Methodology for Design of Emulsion Based Chemical Products

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
Authors: Mattei, M. (Intern), Kontogeorgis, G. (Intern), Gani, R. (Intern)
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PSE_2012_Poster.pdf
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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 poroposed to reduce the number of slimtube simulations needed. In addition, it is also discussed how to parallelize slimtube simulations for modem computers with multiple CPU cores to further chop the computation time. Copyright 2012, Society of Petroleum Engineers.

General information
State: Published
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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Publisher: Society of Petroleum Engineers
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.
Colloid Transport and Retention: Recent Advances in Colloids Filtration Theory

Book Description: Colloidal science and technology is one of the fastest growing research and technology areas. This book explores the cutting edge research in colloidal science and technology that will beusefull in almost every aspect of modern society. This book has a depth of information related to historical prospective, synthesis, characterization, theoretical modeling and application of unique class of colloidal materials starting from colloidal gold to coated silica colloid and platinum, titania colloids. This book is unique in its design, content, providing depth of science about different colloidal materials and their applications in chemistry, physics, biological, medical sciences and environment. Graduate students, academic and industrial researchers and medical professionals will discover recently developed colloidal materials and their applications in many areas of human endeavors through this book.

General information
State: Published
Organisations: Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Ressources Engineering
Authors: Yuan, H. (Intern), Shapiro, A. (Intern)
Publication date: 2012
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.
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® (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.
Corrigendum to "Thermodynamic modeling of phase equilibria of semi-clathrate hydrates of CO$_2$, CH$_4$, or N$_2$+tetra-n-butylammonium bromide aqueous solution" [Chem. Eng. Sci. 81 (2012) 319–328]
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 CO₂ solubility study using the apparatus based on the synthetic method; CO₂ solubility in aqueous solutions of the potassium salts of L-lysine and L-proline, with concentrations of 3.5 molal and 7 molal respectively, were studied at CO₂ 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 CO₂ partial pressures up to around 2.3 MPa.
Chapter 8, concludes on the accomplishments of the project, and finally addresses considerations concerning future work.

General information
State: Published
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Crystallization Kinetics Identification within a Generic Modeling Framework

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Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Center for Energy Resources Engineering, CERE – Center for Energy Resources Engineering, Center for Process Engineering and Technology
Authors: Meisler, K. T. (Intern), Abdul Samad, N. A. F. B. (Intern), von Solms, N. (Intern), Gernaey, K. (Intern), Gernaey, K. (Intern)
Number of pages: 2
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Design of an Emulsified Hand Wash Through a Systematic Model-Based Methodology

General information
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Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Center for Energy Resources Engineering, CERE – Center for Energy Resources Engineering, Columbia University
Authors: Mattei, M. (Intern), Hill, M. (Ekstern), Kontogeorgis, G. (Intern), Gani, R. (Intern)
Number of pages: 2
Publication date: 2012
Main Research Area: Technical/natural sciences
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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 using 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 those parameters are checked using a quality assessment algorithm which combines four widely used consistency tests (Herinton, 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.
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.

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), Ilani-Kashkouli, P. (Ekstern), Mohammadi, A. H. (Ekstern), Ramjugernath, D. (Ekstern), Richon, D. (Intern)
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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
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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
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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
BFI (2009): BFI-level 2
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
Highlights:
- A data set consisting of 1672 viscosity values and comprising 443 ILs was collated from the literature.
- A reliable group contribution method has been developed using this dataset.
- The method employs a total of 46 sub-structures in addition to the temperature to predict the viscosity of ILs.
- Twenty four sub-structures related to anions, and 22 sub-structures related cations were implemented.
- The model produces very encouraging results.

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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.
Scopus rating (2015): SJR 1.038 SNIP 1.606 CiteScore 2.96
Web of Science (2015): Indexed yes
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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
BFI (2009): BFI-level 2
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
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Atmospheric pressure, Computer program listings, Crude oil, Patient monitoring, Refractive index, Stability, Support vector machines, Asphaltenes
DOIs: 10.1016/j.ces.2012.06.060

Bibliographical note
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.
Source: dtu
Efficient Iterated Filtering

Parameter estimation in general state space models is not trivial as the likelihood is unknown. We propose a recursive estimator for general state space models, and show that the estimates converge to the true parameters with probability one. The estimates are also asymptotically Cramer-Rao efficient. The proposed estimator is easy to implement as it only relies on non-linear filtering. This makes the framework flexible as it is easy to tune the implementation to achieve computational efficiency. This is done by using the approximation of the score function derived from the theory on Iterative Filtering as a building block within the recursive maximum likelihood estimator.

General information
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Authors: Lindström, E. (Ekstern), Ionides, E. (Ekstern), Frydendall, J. (Intern), Madsen, H. (Intern)
Pages: 1785-1790
Publication date: 2012

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(trifluoromethylsulfonyl)imide ([C2mim][NTf2]) and 1-butyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide([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.

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 do Porto
Authors: Maia, F. M. (Ekstern), Tsivintzelis, I. (Intern), Rodriguez, O. (Ekstern), Macedo, E. A. (Ekstern), Kontogeorgis, G. (Intern)
Pages: 128-143
Erratum to: Transport properties of natural gas through polyethylene nanocomposites at high temperature and pressure

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BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
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Scopus rating (2016): SJR 0.429 SNIP 0.594 CiteScore 1.39
BFI (2015): BFI-level 1
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ISI indexed (2013): ISI indexed yes
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Scopus rating (2012): SJR 0.703 SNIP 1.267 CiteScore 2.09
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Scopus rating (2011): SJR 0.523 SNIP 1.255 CiteScore 1.67
ISI indexed (2011): ISI indexed yes
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Scopus rating (2010): SJR 0.516 SNIP 0.717
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.654 SNIP 0.815
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.541 SNIP 0.809
Scopus rating (2007): SJR 0.493 SNIP 0.649
Scopus rating (2006): SJR 0.334 SNIP 0.568
Estimating filtration coefficients for straining from percolation and random walk theories

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

The Leverage 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.

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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.

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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 (H₂S), and carbon dioxide (CO₂) 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 H₂S 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.

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- Web of Science (2011): Indexed yes
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- Web of Science (2007): Indexed yes
- Scopus rating (2006): SJR 1.034 SNIP 1.245
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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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.

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.
Higher alcohols synthesis from syngas over carbon-nanotube supported Iron-Chromium catalysts

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Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre, CERE – Center for Energy Ressources Engineering, Center for Electron Nanoscopy, Technical University of Denmark, Haldor Topsoe AS
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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.

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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 alkanolamies, 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.
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 SO$_4^{2-}$, Ca$^{2+}$, and 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.

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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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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 gasses. 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.

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.
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.

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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
Phase Equilibria of Three Binary Mixtures: Methanethiol + Methane, Methanethiol + Nitrogen, and Methanethiol + Carbon Dioxide

New vapor-liquid equilibrium (VLE) data for methanethiol (MM) + methane (CH$_4$), methanethiol (MM) + nitrogen (N$_2$), and methanethiol (MM) + carbon dioxide (CO$_2$) 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).
**General information**

State: Published

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

Authors: Awan, J. (Intern), Tsivintzelis, I. (Intern), Coquelet, C. (Ekstern), Kontogeorgis, G. (Intern)

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**Publication information**

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- 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
- Web of Science (2003): Indexed yes
Phase equilibrium modeling of gas hydrate systems for CO\textsubscript{2} capture

Two thermodynamic models capable of describing dissociation pressures of mixed gas clathrate hydrates formed from ternary mixtures of CO\textsubscript{2}, N\textsubscript{2}, 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 CO\textsubscript{2} 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 CO\textsubscript{2} 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 CO\textsubscript{2} below 0.12 to 0.16 (depending on temperature) to structure I hydrates at mole fractions of CO\textsubscript{2} above this concentration range. The exact transition concentration is shown to increase with increasing temperature. Model II predicts mixed hydrate equilibrium pressures to be stable in concentrations down to vapor phase mole fractions of CO\textsubscript{2} 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.
Process simulation of CO₂ 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 CO₂. 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 \( \text{CO}_2-\text{NH}_3-\text{H}_2\text{O} \) 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.

**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, DONG Energy A/S

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- BFI (2016): BFI-level 1
- Scopus rating (2016): CiteScore 4.38 SJR 1.345 SNIP 1.536
- Web of Science (2016): Indexed yes
- BFI (2015): BFI-level 1
- Scopus rating (2015): SJR 1.515 SNIP 1.537 CiteScore 4.37
- BFI (2014): BFI-level 1
- Scopus rating (2014): SJR 2.06 SNIP 2.412 CiteScore 4.95
- Web of Science (2014): Indexed yes
- BFI (2013): BFI-level 1
- Scopus rating (2013): SJR 2.331 SNIP 3.018 CiteScore 5.66
- ISI indexed (2013): ISI indexed yes
- Web of Science (2013): Indexed yes
- BFI (2012): BFI-level 1
- Scopus rating (2012): SJR 1.302 SNIP 1.987 CiteScore 4.7
- ISI indexed (2012): ISI indexed yes
- Web of Science (2012): Indexed yes
- BFI (2011): BFI-level 1
- Scopus rating (2011): SJR 2.499 SNIP 2.633 CiteScore 6.61
- ISI indexed (2011): ISI indexed yes
- Web of Science (2011): Indexed yes
- BFI (2010): BFI-level 1
- Scopus rating (2010): SJR 1.481 SNIP 2.436
- Web of Science (2010): Indexed yes
- BFI (2009): BFI-level 1
- Scopus rating (2009): SJR 2.058 SNIP 2.589
- BFI (2008): BFI-level 1
- Scopus rating (2008): SJR 0.599 SNIP 1.172

Original language: English

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 (T_d) data for ionic liquids (ILs). A data set consisting of T_d 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 T_d 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, 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)
Pages: 557-563
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Ratings:
BFI (2018): BFI-level 2
BFI (2017): BFI-level 2
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
BFI (2009): BFI-level 2
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
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Source: dtu
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.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre, Center for Energy Resources Engineering, CERE – Center for Energy Resources Engineering, Swiss Federal Institute of Technology
Authors: Beier, M. J. (Intern), Grunwaldt, J. (Intern), Tsivintzelis, I. (Intern), Jensen, A. D. (Intern), Kontogeorgis, G. M. (Intern), Baiker, A. (Ekstern)
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Main Research Area: Technical/natural sciences

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BFI (2018): BFI-level 2
BFI (2017): BFI-level 2
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.01 SJR 0.976 SNIP 1.266
Web of Science (2016): Indexed yes
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
Web of Science (2012): Indexed yes
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
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 an 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.

General information
State: Published
Organisations: Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering
Authors: Fosbøl, P. L. (Intern), Maribo-Mogensen, B. (Intern), Thomsen, K. (Intern)
Pages: 844-859
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Main Research Area: Technical/natural sciences

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Journal: Energy Procedia
Volume: 37
ISSN (Print): 1876-6102
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
BFI (2016): BFI-level 1
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.

General information

State: Published
Organisations: Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Ressources Engineering, Delft University of Technology, MINES ParisTech, Eindhoven University of Technology
Authors: Kazemi, S. (Ekstern), Belandria, V. (Ekstern), Janssen, N. (Ekstern), Richon, D. (Intern), Peters, C. J. (Ekstern), Kroon, M. C. (Ekstern)
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Main Research Area: Technical/natural sciences

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Journal: Journal of Supercritical Fluids
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BFI (2018): BFI-level 2
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.

**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 Ressources Engineering
Authors: Abdul Samad, N. A. F. B. (Intern), Meisler, K. T. (Intern), Gernaey, K. (Intern), von Solms, N. (Intern), Gani, R. (Intern)
Pages: 945-949
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Crystallization, Generic modelling, Model identification, Data handling
Source: dtu
Source-ID: u::4487
Publication: Research - peer-review › Article in proceedings – Annual report year: 2012

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.

**General information**
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Organisations: Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Ressources Engineering, Duke Clinical Research Institute
Authors: Fosbøl, E. L. (Ekstern), Fosbøl, P. L. (Intern), Harrington, R. A. (Ekstern), Eapen, Z. J. (Ekstern), Peterson, E. D. (Ekstern)
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Publication date: 2012
Main Research Area: Technical/natural sciences

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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
Thermally induced permeability reduction due to particle migration in sandstones: the effect of temperature on kaolinite mobilisation and aggregation
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 hydroxyccinnamate saccharide ester synthesis in organic solvent systems as well as other enzymatic hydroxyccinnamate 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 CO₂, CH₄, or N₂+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 CO₂, CH₄, or N₂+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
Authors: Eslamimanesh, A. (Ekstern), Mohammadi, A. H. (Ekstern), Richon, D. (Intern)
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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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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.

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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 (CH₃SH) + methane (CH₄) + water (H₂O) 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 CH₃SH 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 CH₄ 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 CH₃SH 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 CH₃SH in all phases, particularly the vapor phase.
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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 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.

General information


Investigation and Modelling of Diesel Hydrotreating Reactions

This project consists of a series of studies, that are related to hydrotreating of diesel. Hydrotreating is an important refinery process, in which the oil stream is upgraded to meet the required environmental specifications and physical properties. Although hydrotreating is a mature technology it has received increased attention within the last decade due to tightened legislations regarding the sulfur content, e.g. the demand for Ultra Low Sulfur Diesel (ULSD) with a maximum sulfur content of as low as 10 ppm S has increased. The process is complex, as the performance of a hydrotreating reactor is governed by intrinsic kinetics, diffusion in the pores of the catalyst, mass transfer between the phases and the equilibrium between the gas and the liquid phase. In order to optimize the process and develop better simulation tools, a detailed understanding of the different processes and phenomena is needed. The hydrogenation of aromatics during hydrotreating is important, as the aromatics content of the product influences the properties of the product, and since the conversion is important for the hydrogen consumption. It is well-known that saturation of fused aromatic rings can be limited by thermodynamic equilibrium at typical industrial hydrotreating conditions. Equilibrium constants have been calculated based on experimental measurements for the hydrogenation of naphthalene and phenanthrene. The kinetics of hydrogenation of a model compound, naphthalene, has been studied on a commercial CoMo catalyst, and a simple kinetic model is presented. Hydrogenation of fused aromatic rings are known to be fast, and it is possible, that the reaction rates are limited by either internal or external mass transfer. An experiment conducted at industrial temperatures and pressure, using naphthalene as a model compound, have shown, that intra-particle diffusion resistance are likely to limit the reaction rate. In order to produce ULSD it is necessary to remove sulfur from some of the most refractive sulfur compounds, such as sterically hindered dibenzothiophenes. Basic nitrogen compounds are known to inhibit certain hydrotreating reactions. Experimental results are presented, showing the effect of 3 different nitrogen compounds, acridine, 1,4-dimethylcarbazole and 3-methylindole, on the hydrodesulfurization of a real feed and of a model compound, 4,6-dimethylphenothiophene. It is shown, that a basic nitrogen compound is the strongest inhibitor, and that it not only inhibits the hydrodesulfurization reaction, but also the hydrodenitrogenation of other nitrogen compounds. The nitrogen compounds are shown to mainly inhibit the hydrogenation pathway rather than the direct desulfurization route due to a stronger adsorption on hydrogenation sites. Since feeds used in the hydrotreating process, usually gas-oils, are complex mixtures with a large number of compounds, analysis of the reactions of individual compounds can be difficult. In this work a model-diesel feed consisting of 13 different compounds, representing the most important component classes, has been hydrotreated on a commercial NiMo catalyst. The difference of the reactivity and behavior of the different compounds in the mixture have been investigated. A steady-state trickle-bed reactor model has been set-up. The heterogeneous model considers co-current flow of two fluid phases, gas and liquid. The model takes internal and external mass transfer into account. It considers mass transfer between the 2 fluid phases (gas and liquid), and the equilibrium between them. As reactor models is becoming an important tool to understand the process, detailed kinetic models are needed in order to simulate hydrotreating of complex mixtures. A Robinson-Mahoney reactor is a three-phase reactor that behaves as a continuous stirred tank reactor, and therefore allows for the direct measurement of reaction rates, which can be used to develop kinetic models. Hydrogenation reactions are quite fast, and in order to avoid mass transfer limitations, and only measure intrinsic rates, experiments are often conducted, at conditions that are milder than in industrial units. A reactor model for a Robinson-Mahoney reactor that takes mass transfer into account is presented, and it has been used to test a set of kinetic models at industrial conditions.
**Extension of association models to complex chemicals**

Summary of "Extension of association models to complex chemicals". Ph.D. thesis by Ane Søgaard Avlund. The subject of this thesis is the application of SAFT type equations of state (EoS). Accurate and predictive thermodynamic models are important in many industries including the petroleum industry. The SAFT EoS was developed 20 years ago, and a large number of papers on the subject has been published since, but many issues still remain unsolved. These issues are both theoretical and practical. The SAFT theory does not account for intramolecular association, it can only treat flexible chains, and does not account for steric self-hindrance for tree-like structures. An important practical problem is how to obtain optimal and consistent parameters. Moreover, multifunctional associating molecules represent a special challenge. In this work two equations of state using the SAFT theory for association are used; CPA and sPC-SAFT. Phase equilibrium and monomer fraction calculations with sPC-SAFT for methanol are used in the thesis to illustrate the importance of parameter estimation when using SAFT. Different parameter sets give similar pure component vapor pressure and liquid density results, whereas very different mixture results are obtained. The performance of the theory, therefore, depends significantly on the parameter estimation, and this is important to consider if different theories (or association schemes) are compared. The CPA EoS has been applied for alkanolamines, as a continuation of previous study, were only the simple 2 (1:1) and 4 (2:2) association schemes were investigated. It is in this work investigated for MEA (monoethanolamine) how the results with CPA is effected if a more advanced association scheme is used, where different association parameters are used for the different functional groups. It is also tested whether increasing the number of sites for DEA (diethanolamine) improves the results. It can be shown from experimental data that intramolecular association is dominating compared to intermolecular association in certain systems, and that the intramolecular association can significantly alter the phase behavior of a mixture. Lattice theories have earlier on been extended to include intramolecular association for polyethoxyalcohols, while SAFT has only been extended to intramolecular association for chains with 2 associating sites. A general theory for intramolecular association is presented in the thesis, and compared to the corresponding lattice theory. The theory for intramolecular association is then applied in connection with sPC-SAFT for mixtures containing glycol ethers. Calculations with sPC-SAFT (without intramolecular association) are presented for comparison, and the results with sPC-SAFT are moreover compared to results with CPA and SAFT-HS. The comparisons show that while the improved theory does improve the predictive performance of the model, the choice of association scheme and the parameter estimation are at least as important. In general it is found in this project that the parameter estimation is very important for the performance of a SAFT EoS, and that emphasis should be put on that area as well as on improving the theory.

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**Migration of plasticisers from PVC and other polymers**

The main purpose of this thesis is to investigate, from a modeling point of view, the migration of GRINDSTEDr SOFT-N-SAFE (SNS) and other plasticisers from polyvinyl chloride (PVC) and polyolefin food package materials and into foodstuff (specifically the four food simulants set by EU legislation). In this work it is shown how diffusion coefficients can be obtained by regression of experimental migration data plotted as the square root of time. This was done from plasticiser migration data of GRINDSTEDr SOFT-N-SAFE, GRINDSTEDr ACETEM 95 CO (Acetem) and Epoxidised Soybean Oil (ESBO) migrating from Polyvinyl Chloride (PVC) and into iso-octane at 20°C, 40°C and 60°C. Using these experimentally obtained diffusion coefficients the migration was modeled using two analytical models with relatively good accuracy. The diffusion coefficient in highly plasticised PVC should, however, not be considered uniform over the whole polymer layer.
when the migrant is the plasticiser itself. It was attempted to predict the diffusion coefficient of SNS in highly plasticised PVC from pure component data alone, using the model by Vrentas and Vrentas, which is based on the free volume theory. The results, however, showed that the model under-predicts the experimental diffusion coefficient values. These experimentally obtained values should be regarded as average diffusion coefficient values of the whole polymer and lower than the diffusion coefficient of the fully plasticised PVC. Instead of using this elaborated complex model, it was decided to use the much simpler semi-empirical model by Piringer. Using this simple model, with a polymer-specific parameter obtained from ESBO migration data alone, it was possible to estimate diffusion coefficients for Acetem and SNS. The results were close to the experimentally obtained diffusion coefficients at 20 °C, except at higher temperatures. Using the finite element mesh method in Matlab and COMSOL environments the migration was modeled with a diffusion coefficient able to change with local plasticiser concentration. Three different models for this plasticiser concentration dependence of the diffusion coefficient were evaluated. All models performed similarly, with better predicting ability compared to modeling with a static diffusion coefficient. This numerical solution by the finite element mesh method has also been used to model the migration of an antistatic additive to the surface of Low Density Polyethylene (LDPE) and Poly Propylene (PP). It was possible with a newly developed model to estimate the migration with very high accuracy. This result leads to the somewhat surprising conclusion that the controlling step in the migration of the additive to the surface was not the migration within the polymer bulk. Migration is probably due to a temperature dependent partitioning of the additive between the polymer bulk and the surface layer. The possibility of using molecular dynamics calculations to estimate the partition coefficients of additives between polymers and foodstuff was also investigated. The development of the methodology was done against experimental data of a system composed of a hydrophilic or a hydrophobic additive between LDPE and different ethanol/water mixtures. The calculated partition coefficients of different additives between LDPE and ethanol/water were correlated with high accuracy against experimental data. To extend the methodology to acetic acid systems (food simulant B), it was chosen firstly to investigate the predictive capabilities of the TraPPE, OPLS-AA and CHARMM27 force fields for pure acetic acid and acetic acid / water mixtures. None of the three force fields was able to predict satisfactorily the density of acetic acid / water mixtures. Only the CHARMM27 force field was able to predict the local density maxima of the system. A hydrogen bond connectivity counting code was developed for investigating the clustering of acetic acid. Statistics using the cluster counting code showed that the acetic acid molecules in the liquid phase mostly formed chain-like structures, with chains of 2 and 3 molecules in size to be the most predominant ones. Furthermore, the ability of the force fields to predict the enthalpy of vaporization was tested. All three force fields over-predict this property, resulting to a value about twice the experimental one (50kJ/mol compared to 23.7kJ/mol). The gas phase consisted almost entirely of monomers, where experimental Pressure-Volume data of the gas phase at 298K and 1 bar give a dimer fraction of around 80-90%. This dimer fraction in the gas phase was elevated using higher atomic charges as shown by Chocholousova et al.[J. Chocholousova, J. Vacek, and P. Hobza; J. Phys. Chem. A; 107, 17, (2003), 3086-3092], but the calculated enthalpy of vaporization was still almost twice as high. It was shown that most literature data listing a value of 50kJ/mol originate from the work by Konicek and Wadsö[J. Konicek and I. Wadsö; Acta Chem. Scand.; 24, 7, (1970), 2612-2616] from 1970. In the same work is explained how the enthalpy of vaporization of acetic acid theoretically can be seen as consisting of two contributions, the "pure" enthalpy of vaporization of the monomer and the enthalpy of dissociation. It is important that this theoretically-derived "pure"enthalpy of vaporization (which is 50kJ/mol) is not confused with the experimentally obtained enthalpy of vaporization (23.7kJ/mol). The OPLS-AA force field is parameterized towards the theoretical "pure" enthalpy of vaporization in a correct way, by only calculating the energy difference for the single acetic acid monomer molecule between the two phases. However simulations in this work have shown that these parameters do not allow the force field to predict the gas phase dimer fraction accurately. Overall from this work it can be concluded that a full prediction of migration in polyolefins can be obtained using the numerical solution by finite element mesh together with diffusion coefficients obtained from the Piringer model and partition coefficient by molecular dynamics. For the complex system of migration of plasticisers in highly plasticised PVC, a full predictive model was not obtained. A model was, however, developed for this system that predicts satisfactorily with only 1 or 2 adjustable parameters to plasticiser migration from PVC.

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Advanced Waterflooding in Chalk Reservoirs: Crude Oil/Brine Interaction Study

Over the last decade, a number of studies have shown SO₄²⁻, Ca²⁺ and Mg²⁺ 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.

Advanced waterflooding in chalk reservoirs: Understanding of underlying mechanisms

Over the last decade, a number of studies have shown SO₄²⁻, Ca²⁺ and Mg²⁺ 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 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.
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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.

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An Explanation of the Selective Plating of Laser Machined Surfaces using Surface Tension Components

General information
State: Published
Organisations: Department of Mechanical Engineering, CERE – Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering
Authors: Zhang, Y. (Intern), Kontogeorgis, G. (Intern), Hansen, H. N. (Intern)
Pages: 2101-2111
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Publication information
Journal: Journal of Adhesion Science and Technology
Volume: 25
ISSN (Print): 0169-4243
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 0.362 SNIP 0.591 CiteScore 1.03
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.355 SNIP 0.637 CiteScore 0.99
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.4 SNIP 0.664 CiteScore 1.05
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.437 SNIP 0.769 CiteScore 1.19
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Two association models, the CPA and sPC-SAFT equations of state, are applied to binary mixtures containing alkanolamines and hydrocarbons or water. CPA is applied to mixtures of MEA and DEA, while sPC-SAFT is applied to MEA–n-heptane liquid–liquid equilibria and MEA–water vapor–liquid equilibria. The role of association schemes is investigated in connection with CPA, while for sPC-SAFT emphasis is given on the role of different types of data in the determination of pure compound parameters suitable for mixture calculations. Moreover, the performance of CPA and sPC-SAFT for MEA-containing systems is compared. The investigation showed that vapor pressures and liquid densities were not sufficient for obtaining reliable parameters with either CPA or sPC-SAFT, but that at least one other type of information is needed. LLE data for a binary mixture of the associating component with an inert compound is very useful in the estimation. The simple 4-site scheme is suitable for both CPA and sPC-SAFT and little is gained by using more complex association schemes. Finally, the results of CPA and sPC-SAFT are overall similar and whatever differences are seen appear to be more related to details in the parametrization rather than the different functional forms of the two equations of state.

General information
State: Published
Organisations: CERE – Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, Administration
Authors: Avlund, A. S. (Intern), Eriksen, D. K. (Intern), Kontogeorgis, G. (Intern), Michelsen, M. L. (Intern)
Pages: 31-37
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Main Research Area: Technical/natural sciences

Publication information
Journal: Fluid Phase Equilibria
Volume: 306
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ISSN (Print): 0378-3812
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 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
DEA, sPC-SAFT, VLE, LLE, CPA, Alkanolamine
DOIs: 10.1016/j.fluid.2011.02.005
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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Organisations: CERE – Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, Administration, Center for Energy Resources Engineering
Pages: 5088-5093
Publication date: 2011
Main Research Area: Technical/natural sciences

Publication information
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Volume: 56
Issue number: 12
ISSN (Print): 0021-9568
Ratings:
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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
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
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.
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.

Chemical Absorption Materials
Chemical absorption materials that potentially can be used for post combustion carbon dioxide capture are discussed. They fall into five groups, alkanolamines, alkali carbonates, ammonia, amino acid salts, and ionic liquids. The chemistry of the materials is discussed and advantages and drawbacks are mentioned. References to review papers, papers with experimental data, and papers describing the thermodynamic modelling of the systems are given.
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
State: Published
Organisations: CERE – Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, Department of Chemistry, Center for Energy Resources Engineering, DONG Energy A/S
Authors: Darde, V. C. A. (Intern), van Well, W. J. (Ekstern), Stenby, E. H. (Intern), Thomsen, K. (Intern)
Pages: 1443-1450
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Conference: 10th International Conference on Greenhouse Gas Control Technologies : GHGT-10, Amsterdam, 01/01/2011
Main Research Area: Technical/natural sciences

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Volume: 4
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BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.16 SJR 0.467 SNIP 0.586
Web of Science (2016): Indexed yes
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
Scopus rating (2010): SJR 0.433 SNIP 0.957
Web of Science (2009): Indexed yes
Original language: English
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DOIs:
10.1016/j.egypro.2011.02.010
Source: orbit
Source-ID: 285841
Publication: Research - peer-review › Conference article – Annual report year: 2011
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.
chemicals in oil-water systems. Traditionally distribution of chemicals in oil-water system 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 methane 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 alkane + 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.

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: Riaz, M. (Intern), Kontogeorgis, G. (Intern), Stenby, E. H. (Intern), Yan, W. (Intern)
Number of pages: 189
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Publication information
Place of publication: Kgs.Lyngby
Publisher: Technical University of Denmark, Department of Chemical Engineering
Original language: English
Main Research Area: Technical/natural sciences
Electronic versions:
Source: dtu
Source-ID: u::3692
Dynamic flow method to study the CO2 loading capacity of amino acid salt solutions

Due to a number of advantages amino acid salt solutions have emerged as alternatives to the alkanolamine solvents for the chemical absorption of CO2 from flue gas. The use of amino acids in CO2 capture is a bio-mimetic process, as it is similar to CO2 binding by proteins in the blood, such as hemoglobin. Amino acid salt solutions have the same amine functionality as alkanolamines, and are thus expected to behave similar towards CO2 in flue gas. Despite rising interest, few studies have been performed so far on amino acids as CO2 absorbents.

Estimation of Chromatographic Columns Performances using Computer Tomography and CFD Simulations

The flow inside a chromatographic column depends decisively on the packed bed inside. Non-destructive X-ray computed tomography (CT) was applied as a novel measurement technique to visualize the distribution of velocity and axial dispersion coefficients in preparative scale columns. The results show, that spherical particles seem to be more efficient than irregular ones in terms of HETP, which has to be partly a result of the more homogeneous flow profile they induce. The prediction of column performance in dependence of the structure of the packed bed was simulated by CFD (Computational Fluid Dynamics), using a model which besides the hydrodynamics parameters attained by CT also includes adsorption isotherms and mass transfer parameters. The results of the CFD simulation shall help to establish rules for selecting the right adsorption material for a given separation task in advance.
Evaluation of the CO2 Behavior in Binary Mixtures with Alkanes, Alcohols, Acids and Esters Using the Cubic-Plus-Association Equation of State

General information
State: Published
Organisations: CERE – Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering
Authors: Oliveira, M. B. (Ekstern), Queimada, A. J. (Ekstern), Marrucho, I. M. (Ekstern), Kontogeorgis, G. (Intern), Coutinho, J. A. P. (Ekstern)
Pages: 876-892
Publication date: 2011
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Supercritical Fluids
Volume: 55
ISSN (Print): 0896-8446
Ratings:
BFI (2018): BFI-level 2
BFI (2017): BFI-level 2
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.01 SJR 0.976 SNIP 1.266
Experimental Determination and Modeling of the Phase Behavior for the Selective Oxidation of Benzyl Alcohol in Supercritical CO2

In this study the phase behavior of mixtures relevant to the selective catalytic oxidation of benzyl alcohol to benzaldehyde by molecular oxygen in supercritical CO2 is investigated. Initially, the solubility of N2 in benzaldehyde as well as the dew points of CO2–benzyl alcohol–O2 and CO2–benzaldehyde–water ternary mixtures were experimentally determined. The cubic plus association (CPA) equation of state was used to model the phase behavior of the experimentally investigated systems as well as the phase behavior of relevant mixtures that can exist inside the reactor during the reaction time. In this direction, the CPA binary interaction parameters were estimated from the corresponding binary systems and the phase behavior of two ternary systems, i.e. CO2–benzyl alcohol–O2 (reacting mixture) and CO2–benzaldehyde–water (mixture of products) as well as the phase behavior of multicomponent mixtures containing both reactants and products were predicted. CPA was proved to be a versatile model that can predict the complex phase behavior of the aforementioned systems. The results reveal that the ternary mixture of products (CO2–benzaldehyde–water) and the intermediate multicomponent mixtures containing both products and reactants require lower pressure than the
corresponding mixture of the reactants (CO2–benzyl alcohol–O2) in order to be in a single phase.

**General information**

State: Published
Organisations: CERE – Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, CHEC Research Centre, Swiss Federal Institute of Technology
Authors: Tsivintzelis, I. (Intern), Beier, M. J. (Intern), Grunwaldt, J. (Intern), Baiker, A. (Ekstern), Kontogeorgis, G. (Intern)
Pages: 83-92
Publication date: 2011
Main Research Area: Technical/natural sciences

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Ratings:
BFI (2018): BFI-level 2
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
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
State: Published
Organisations: CERE – Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, Department of Chemistry, Center for Energy Resources Engineering, DONG Energy A/S
Authors: Darde, V. C. A. (Intern), van Well, W. J. (Ekstern), Fosbøl, P. L. (Intern), Stenby, E. H. (Intern), Thomsen, K. (Intern)
Pages: 1149-1162
Publication date: 2011
Main Research Area: Technical/natural sciences

Publication information
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Ratings:
BFI (2018): BFI-level 2
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 4.38 SJR 1.345 SNIP 1.536
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.515 SNIP 1.537 CiteScore 4.37
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 2.06 SNIP 2.412 CiteScore 4.95
Web of Science (2014): Indexed yes
**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.

**General information**

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

Authors: Yuan, H. (Intern), Shapiro, A. (Intern)

Publication date: 2011

Event: Poster session presented at Third International Conference on Porous Media, Bordeaux, France, .

Main Research Area: Technical/natural sciences

hyperexponential deposition, porous media, filtration, non-Fickian transport

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**Freezing Point Depression of Aqueous Solutions of DEEA, MAPA and DEEA-MAPA with and without CO2 Loading**

**General information**

State: Published

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

Authors: Waseem Arshad, M. (Intern), Thomsen, K. (Intern)

Publication date: 2011
Freezing Point Depressions of Aqueous MEA, MDEA, and MEA–MDEA Measured with a New Apparatus

Freezing points for aqueous monooethanolamine (MEA), methyl diethanolamine (MDEA), and MEA–MDEA solutions were measured in the concentration range from 0 to 0.4 mass fractions of the alkanolamines. For the aqueous MEA–MDEA system, freezing points for 1:4, 1:2, 1:1, 2:1, and 4:1 molar ratios of MEA/MDEA were determined. The experimental values indicate that the MDEA–water interaction is stronger than the MEA–water interaction. Measurements were carried out by a new modified Beckmann apparatus, which has not previously been described. The apparatus and method proved to have good repeatability and accuracy. A correlation of the freezing points as functions of the solution composition was made. Measurements of aqueous MEA and aqueous MDEA were compared to experiments found in the open literature.
Generic Model and Data Based Framework for Analysis and Development of Crystallization Processes

Heterogeneously Catalyzed Oxidation Reactions Using Molecular Oxygen

Heterogeneously catalyzed selective oxidation reactions have attracted a lot of attention in recent time. The first part of the present thesis provides an overview over heterogeneous copper and silver catalysts for selective oxidations in the liquid phase and compared the performance and catalytic properties to the widely discussed gold catalysts. Literature results were summarized for alcohol oxidation, epoxidation, amine oxidation, phenol hydroxylation, silane and sulfide oxidation, (side-chain) oxidation of alkyl aromatic compounds, hydroquinone oxidation and cyclohexane oxidation. It was found that both copper and silver can function as complementary catalyst materials to gold showing different catalytic properties and being more suitable for hydrocarbon oxidation reactions. Potential opportunities for future research were outlined. In an experimental study, the potential of silver as a catalyst for the selective oxidation of alcohols was investigated. By using a...
straightforward screening approach, silver supported on silica prepared by impregnation was found to be catalytically active in a mixture with nano-sized ceria. The collaborative effect between ceria and silver was traced back to direct physical contact while leaching could be excluded. The silver catalyst was most active when calcined over a short time at 500 °C potentially due to the formation of silver-oxygen species. Removal of these species might be a deactivation mechanism as was suggested by X-ray absorption spectroscopy (XAS) analysis. XAS revealed that silver was in the metallic state. Silver particle sizes estimated from XAS were significantly smaller (2- 3 nm) than from transmission electron microscopy (TEM) and X-ray diffraction (XRD; ca. 30 nm). It was proposed that silver-oxygen species might cause local disorder which would lead to an underestimated particle size by XAS. Based on catalytic studies, a simplified preliminary mechanism was proposed following the dehydrogenation mechanism over gold and palladium catalysts. Comparison of the performance of the silver catalyst with commercial palladium and gold catalysts revealed that all catalysts were more active in combination with ceria nanoparticles and that under the tested reaction conditions silver was equally or even more efficient than the gold catalysts. Calcination at 900 °C of silver on silica prepared by impregnation afforded a catalyst which was used in the selective side chain oxidation. Toluene, p-xylene, ethylbenzene and cumene were oxidized to the corresponding hydroperoxides, alcohols, carbonyl compounds and carboxylic acids most likely following a radical autoxidation mechanism. p-Xylene conversion was promoted by ceria nanoparticles in combination with a carboxylic acid resulting in TONs of up to 2000. In the absence of the carboxylic acid, ceria inhibited the reaction exhibiting radical scavenger properties. Contrary to p-xylene, neither ethylbenzene nor cumene conversion was promoted by ceria even in the presence of a carboxylic acid. Substantial leaching of silver was observed with the impregnated silver catalyst. By using silver supported on CeO2-SiO2 prepared by flame spray pyrolysis, leaching could be limited significantly. XAS investigation revealed that the active catalyst is most likely metallic silver. Compared to silver on silica calcined at 500 °C (vide supra) the particle size obtained from XAS for the impregnated catalyst calcined at 900 °C (> 5 nm) was in qualitative agreement with TEM and XRD results. Oxidation reactions like the previously described alcohol oxidation can profit from the use of pressurized CO2 as a solvent. Phase behavior in CO2 containing systems was previously shown to be important for catalytic reactions. Using the Cubic plus Association (CPA) Equation of State the phase behavior of ternary systems consisting of benzyl alcohol – O2 – CO2 and benzaldehyde – H2O – CO2 were modeled. Dew points of the latter system occurred in general at lower pressures than the former. Good agreement between experimental data measured at catalysis-relevant conditions and the model was found. Experimental dew points occurred at (slightly) lower pressures as predicted by the model. The usefulness of the model was further evaluated in a continuous catalytic study with Pd/Ai2O3 as catalyst where the conversion of benzyl alcohol was monitored as a function of pressure. Indeed the reaction rate differed significantly depending on whether the system was mono- or biphasic. The CPA model predictions therefore assist in locating the pressure regime with the highest catalytic activity in a rational manner making extensive trial-and-error experiments unnecessary. Biphasic conditions close to the dew point gave the highest catalytic activity for benzyl alcohol oxidation over Pd/Ai2O3 while rates were lower under single phase conditions. A reason for this behavior might be overoxidation of palladium or blocking of surface sites by byproducts with low solubility under single phase conditions. Under biphasic conditions the substrate was found to accumulate in the reactor (and the overall experimental setup) leading to longer residence times. Compared to alcohol oxidation the epoxidation of olefins with molecular oxygen is more difficult. Using N,N-dimethylformamide (DMF) as a solvent the Co-based metal-organic framework (MOF) STA-12(Co) catalyzed the epoxidation of styrene, (E)- and (Z)-stilbene. While the stilbene isomers were observed with increasing temperature, substrate concentration and oxygen supply while the amount of catalyst only had a limited influence. Some cobalt leaching was observed though the MOF in general exhibited good stability as suggested by scanning electron microscopy (SEM), XRD and XAS. Amines (from DMF) deactivated the catalyst. The MOF catalyst featured an induction period which was not observed with homogeneously dissolved cobalt. During the induction, the catalyst was activated by benzaldehyde forming as a side-product which led to the interesting effect that co-epoxidation of (E)-stilbene proceeded faster in the presence of styrene since styrene is more easily oxidized to benzaldehyde. Further catalytic studies allowed the formulation of a tentative reaction mechanism.

**General information**

*State:* Published  
*Organisations:* Department of Chemical and Biochemical Engineering, CHEC Research Centre, CERE – Center for Energy Ressources Engineering  
*Authors:* Beier, M. J. (Intern), Grunwaldt, J. (Intern), Jensen, A. D. (Intern), Kontogeorgis, G. (Intern)  
*Number of pages:* 204  
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*Publisher:* Technical University of Denmark, Department of Chemical Engineering  
*Original language:* English  
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*Source:* orbit  
*Source-ID:* 313228  
*Publication:* Research › Ph.D. thesis – Annual report year: 2011
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.

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), Shapiro, A. (Intern)
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Journal: Journal of Petroleum Science and Engineering
Volume: 78
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BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.56 SJR 0.764 SNIP 1.631
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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
Inhibition of Structure I and II Gas Hydrates using Synthetic and Biological Kinetic Inhibitors

General information
State: Published
Organisations: CERE – Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering
Authors: Jensen, L. (Intern), Thomsen, K. (Intern), von Solms, N. (Intern)
Pages: 17-23
Publication date: 2011
Main Research Area: Technical/natural sciences

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Journal: Energy & Fuels
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BFI (2018): BFI-level 2
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
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)
Pages: 1759-1769
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Main Research Area: Technical/natural sciences

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Journal: Molecular Physics
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ISSN (Print): 0026-8976
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BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
Leaching from waste incineration bottom ashes treated in a rotary kiln
Leaching from municipal solid waste incineration bottom ash treated in a rotary kiln was quantified using a combination of lab-scale leaching experiments and geochemical modelling. Thermal treatment in the rotary kiln had no significant effect on the leaching of Al, Ba, Ca, Mg, Si, Sr, Zn, sulfate and inorganic carbon. Leaching of these elements from the treated residues remained unchanged and was, in general, controlled by solubility of the same minerals as in the untreated residues. Leaching of Cd, Co, Ni, Ti, Be, Bi, and Sn from both untreated and treated residues was found to be close to or below their detection limits; no effects of the thermal treatment on leachability of these metals were observed. The leaching of Cl, dissolved organic carbon (DOC), Cu and Pb decreased by at least one order of magnitude after the thermal treatment. This could be explained by evaporation (Cl) and by a better burnout of organic matter which then limited metal–DOC complexation and mobility. At the same time, leaching of Mo and Cr appeared to increase by a factor of 4 and
more than two orders of magnitude, respectively. The large changes in Cr leaching may be explained by decreases in Al reduction capacity after the thermal treatment. Overall, rotary kiln thermal treatment of bottom ashes can be recommended to reduce the leaching of Cu, Pb, Cl and DOC; however, increased leaching of Cr and Mo should be expected.

**General information**

State: Published
Organisations: Residual Resource Engineering, Department of Environmental Engineering, CERE – Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, CHEC Research Centre, Babcock & Wilcox Vølund A/S
Authors: Hyks, J. (Intern), Nesterov, I. (Intern), Mogensen, E. (Ekstern), Jensen, P. A. (Intern), Astrup, T. (Intern)
Pages: 995-1007
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Main Research Area: Technical/natural sciences

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- Web of Science (2017): Indexed Yes
- BFI (2016): BFI-level 1
- Scopus rating (2016): CiteScore 1.76 SJR 0.655 SNIP 1.036
- BFI (2015): BFI-level 1
- Scopus rating (2015): SJR 0.617 SNIP 0.899 CiteScore 1.53
- Web of Science (2015): Indexed yes
- BFI (2014): BFI-level 1
- Scopus rating (2014): SJR 0.741 SNIP 1.085 CiteScore 1.28
- Web of Science (2014): Indexed yes
- BFI (2013): BFI-level 1
- Scopus rating (2013): SJR 0.588 SNIP 0.951 CiteScore 1.17
- ISI indexed (2013): ISI indexed yes
- Web of Science (2013): Indexed yes
- BFI (2012): BFI-level 1
- Scopus rating (2012): SJR 0.886 SNIP 1.046 CiteScore 1.4
- ISI indexed (2012): ISI indexed yes
- Web of Science (2012): Indexed yes
- BFI (2011): BFI-level 1
- Scopus rating (2011): SJR 1.027 SNIP 0.865 CiteScore 1.33
- ISI indexed (2011): ISI indexed yes
- Web of Science (2011): Indexed yes
- BFI (2010): BFI-level 1
- Scopus rating (2010): SJR 0.666 SNIP 0.975
- Web of Science (2010): Indexed yes
- BFI (2009): BFI-level 1
- Scopus rating (2009): SJR 0.877 SNIP 1.257
- Web of Science (2009): Indexed yes
- BFI (2008): BFI-level 1
- Scopus rating (2008): SJR 0.49 SNIP 0.933
- Web of Science (2008): Indexed yes
- Scopus rating (2007): SJR 0.352 SNIP 0.666
- Web of Science (2007): Indexed yes
- Scopus rating (2006): SJR 0.295 SNIP 0.755
- Web of Science (2006): Indexed yes
Lipid Processing Technology: Building a Multilevel Modeling Network

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 UNIFACCI model, development of a master parameter table; 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
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Ressources Engineering, Technical University of Denmark, Alfa Laval Copenhagen A/S
Authors: Díaz Tovar, C. A. (Intern), Mustaffa, A. A. (Intern), Mukkerikar, A. (Ekstern), Quaglia, A. (Intern), Kontogeorgis, G. (Intern), Sarup, B. (Ekstern), Gani, R. (Intern)
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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 adoptionanalysis 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 GCPlus 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
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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)
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Lipid Processing Technology: Shifting From Waste Streams to High-Value Commercial by-Products

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Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, CERE – Center for Energy Ressources Engineering, Alfa Laval Copenhagen A/S
Authors: Diaz Tovar, C. A. (Intern), Mustaffa, A. A. (Intern), Kontogeorgis, G. (Intern), Gani, R. (Intern), Sarup, B. (Ekstern)
Publication date: 2011
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Main Research Area: Technical/natural sciences
Measurement and modeling of CO2 solubility in NaCl brine and CO2–saturated NaCl brine density

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Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2011

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 and density.
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 Whilton 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.

**General information**

State: Published  
Organisations: Center for Energy Resources Engineering, CERE – Center for Energy Ressources Engineering, Department of Chemical and Biochemical Engineering, Technical University of Denmark  
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Web of Science (2017): Indexed yes  
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BFI (2015): BFI-level 1  
Scopus rating (2015): SJR 1.515 SNIP 1.537 CiteScore 4.37  
BFI (2014): BFI-level 1  
Scopus rating (2014): SJR 2.06 SNIP 2.412 CiteScore 4.95  
Web of Science (2014): Indexed yes  
BFI (2013): BFI-level 1  
Scopus rating (2013): SJR 2.331 SNIP 3.018 CiteScore 5.66  
ISI indexed (2013): ISI indexed yes  
Web of Science (2013): Indexed yes  
BFI (2012): BFI-level 1  
Scopus rating (2012): SJR 1.302 SNIP 1.987 CiteScore 4.7  
ISI indexed (2012): ISI indexed yes  
Web of Science (2012): Indexed yes  
BFI (2011): BFI-level 1  
Scopus rating (2011): SJR 2.499 SNIP 2.633 CiteScore 6.61  
ISI indexed (2011): ISI indexed yes  
Web of Science (2011): Indexed yes  
BFI (2010): BFI-level 1  
Scopus rating (2010): SJR 1.481 SNIP 2.436  
Web of Science (2010): Indexed yes  
BFI (2009): BFI-level 1  
Scopus rating (2009): SJR 2.058 SNIP 2.589  
BFI (2008): BFI-level 1  
Scopus rating (2008): SJR 0.599 SNIP 1.172

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Measurement, CO2 solubility, Modeling, Brine density, NaCl brine
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
State: Published
Organisations: CERE – Center for Energy Ressources 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), Løkken, T. V. (Ekstern), Solbraa, E. (Ekstern)
Pages: 4342-4351
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Main Research Area: Technical/natural sciences

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Journal: Journal of Chemical and Engineering Data
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Issue number: 12
ISSN (Print): 0021-9568
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BFI (2018): BFI-level 2
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
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, $k_{ij}$, 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, CO$_2$–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 ($k$) and one for the association part ($\beta_{\text{cross}}$). 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 $k_{ij}$ 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 ($\beta_{\text{cross}}$). 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.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering, Center for Energy Resources Engineering
Authors: Breil, M. P. (Intern), Tsivintzelis, I. (Intern), Kontogeorgis, G. (Intern)
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Scopus rating (2016): CiteScore 2.33 SJR 0.869 SNIP 1.155
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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
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
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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
Modeling of the Thermodynamics of the Acetic Acid–Water Mixture Using the Cubic-Plus-Association Equation of State

The cubic-plus-association (CPA) equation of state is applied in this work to mixtures containing acetic acid and water. A previously developed modification of the model, the so-called CPA-Huron–Vidal (CPA-HV), is used. New CPA parameters have been estimated based on the vapor pressure, liquid density, enthalpy of vaporization, and vapor-phase compressibility factor data. The CPA-HV parameters have been fitted to, among others, experimental vapor compressibility factor data and experimental relative volatility data at different temperature ranges. The purpose of the work was to investigate whether the CPA-HV model can describe the vapor–liquid equilibrium for acetic acid–water over a temperature range of 200 K and at the same time represent the behavior of pure acetic acid and acetic acid–water mixtures with respect to enthalpies of vaporization and compressibility factors. It is shown that satisfactory results are overall obtained, but if an excellent match is needed over the whole temperature range, then different interaction parameters need to be used at the various temperature ranges.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering
Authors: Breil, M. P. (Intern), Kontogeorgis, G. (Intern), Behrens, P. K. (Ekstern), Michelsen, M. L. (Intern)
Pages: 5795-5805
Publication date: 2011
Main Research Area: Technical/natural sciences

Publication information
Journal: Industrial & Engineering Chemistry Research
Volume: 50
Issue number: 9
ISSN (Print): 0888-5885
Ratings:
BFI (2018): BFI-level 2
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
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**
State: Published
Organisations: CERE – Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, Department of Chemistry, Center for Energy Resources Engineering
Authors: Tsivintzelis, I. (Intern), Kontogeorgis, G. (Intern), Michelsen, M. L. (Intern), Stenby, E. H. (Intern)
Pages: 38-56
Publication date: 2011
Conference: 20 years of the SAFT equation of state, 01/01/2011
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BFI (2016): BFI-level 2
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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
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
Mutual Solubility of MEG, Water and Reservoir Fluid: Experimental Measurements and Modeling using the CPA Equation of State

This work presents new experimental phase equilibrium data of binary MEG-reservoir fluid and ternary MEG-water-reservoir fluid systems at temperatures 275-326 K and at atmospheric pressure. The reservoir fluid consists of a natural gas condensate from a Statoil operated gas field in the North Sea. Prediction of mutual solubility of water, MEG and hydrocarbon fluids is important for the oil industry to ensure production and processing as well as to satisfy environmental regulations. The CPA equation of state has been successfully applied in the past to well defined systems containing associating compounds. It has also been extended to reservoir fluids in presence of water and polar chemicals using a Pedersen like characterization method with modified correlations for critical temperature, pressure and acentric factor. In this work CPA is applied to the prediction of mutual solubility of reservoir fluid and polar compounds such as water and MEG. Satisfactory results are obtained for mutual solubility of MEG and gas condensate whereas some deviations are observed for the ternary system of MEG-water-gas condensate.

General information
State: Published
Organisations: CERE – Center for Energy Ressources Engineering, Department of Chemical and Biochemical Engineering, Statoil ASA
Authors: Riaz, M. (Intern), Kontogeorgis, G. (Intern), Stenby, E. H. (Intern), Yan, W. (Intern), Haugum, T. (Ekstern), Christensen, K. O. (Ekstern), Solbraa, E. (Ekstern), Løkken, T. V. (Ekstern)
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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
On Application of Non-cubic EoS to Compositional Reservoir Simulation

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.

**General information**

State: Published
Organisations: Center for Energy Resources Engineering, Department of Chemistry, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering
Authors: Yan, W. (Intern), Michelsen, M. L. (Intern), Stenby, E. H. (Intern)
Number of pages: 13
Publication date: 2011
Main Research Area: Technical/natural sciences
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Publication: Research - peer-review › Paper – Annual report year: 2012

**Particles and Pores: New transport and capture mechanisms**

**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), Nielsen, S. M. (Intern), Shapiro, A. (Intern), Stenby, E. H. (Intern)
Publication date: 2011

**Publication information**

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Main Research Area: Technical/natural sciences
Electronic versions:
2011-06-09-CERE_discussion_meeting.pdf

**Bibliographical note**

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Source: orbit
Source-ID: 277564
Publication: Research › Sound/Visual production (digital) – Annual report year: 2011

**Partition Coefficients of Organic Molecules in Squalane and Water/Ethanol Mixtures by Molecular Dynamics Simulations**

Accurate partition coefficient data of migrants between a polymer and a solvent are of paramount importance for estimating the migration of the migrant over time, including the concentration of the migrant at infinite time in the two solvents. In this article it is shown how this partition coefficient can be estimated for both a small hydrophilic and a hydrophobic organic molecules between squalane (used here to mimic low density poly ethylene) and water/ethanol solutes using thermodynamic integration to calculate the free energy of solvation. Molecular dynamics simulations are performed, using the GROMACS software, by slowly decoupling of firstly the electrostatic and then the Lennard–Jones interactions between molecules in the simulation box. These calculations depend very much on the choice of force field. Two force fields have been tested in this work, the TraPPE-UA (united-atom) and the OPLS-AA (all-atom). The computational cheaper TraPPE-UA force field showed to be more accurate over the whole range of systems compared to the OPLS-AA force field. Moreover, some of the calculations were done with five different water models to investigate the influence of the specific water model on the calculations. It was found that the combination of the TraPPE-UA force field and the TIP4p water model gave the best results. Based on the methodology proposed in this article, it is possible to obtain good partition coefficients only knowing the chemical structure of the molecules in the system.
Phase Behavior in EOR Surfactant Flooding

General information
State: Published
Organisations: CERE – Center for Energy Resources 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)
Publication date: 2011
Event: Poster session presented at Thermodynamics 2011, Athens, Greece, .
Main Research Area: Technical/natural sciences
Electronic versions:
prod21322140050111.Thermodynamics_poster_2011[1].pdf
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Source-ID: 313249
Publication: Research - peer-review › Poster – Annual report year: 2011

Phase Equilibrium in Amino Acid Salt Systems for CO2 Capture

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CERE – Center for Energy Ressources Engineering
Authors: Sengeløv, L. W. (Ekstern), Thomsen, K. (Intern)
Publication date: 2011

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Physical mechanisms of deep bed filtration with application to the problems of petroleum industry

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
Authors: Yuan, H. (Intern), Shapiro, A. (Intern), Stenby, E. H. (Intern)
Publication date: 2011

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Pressure Effect on Phase Behavior of Surfactant System

General information
State: Published
Organisations: CERE – Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, Department of Chemistry
Authors: Sanderson, S. B. (Intern), von Solms, N. (Intern), Stenby, E. H. (Intern)
Publication date: 2011
Main Research Area: Technical/natural sciences
Electronic versions:
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Pressure Effect on Phase Behavior of Surfactant System

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Organisations: CERE – Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, Department of Chemistry
Authors: Sanderson, S. B. (Intern), von Solms, N. (Intern), Stenby, E. H. (Intern)
Publication date: 2011
Main Research Area: Technical/natural sciences
Electronic versions:
ESAT_abstract_2011.pdf
Source: orbit
Source-ID: 278468
Publication: Research › Conference abstract for conference – Annual report year: 2011

Properties of cryobrines on Mars
Brines, i.e. aqueous salty solutions, increasingly play a role in a better understanding of physics and chemistry (and eventually also putative biology) of the upper surface of Mars. Results of physico-chemical modeling and experimentally determined data to characterize properties of cryobrines of potential interest with respect to Mars are described. Eutectic diagrams, the related numerical eutectic values of composition and temperature, the water activity of Mars-relevant brines of sulfates, chlorides, perchlorides and carbonates, including related deliquescence relative humidity, are parameters and
properties, which are described here in some detail. The results characterize conditions for liquid low-temperature brines ("cryobrines") to evolve and to exist, at least temporarily, on present Mars. (C) 2010 Elsevier Inc. All rights reserved.
Screening of amino acid salts solutions for application in CO2 capture from flue gas.

Towards Predictive Association Theories
Association equations of state like SAFT, CPA and NRHB have been previously applied to many complex mixtures. In this work we focus on two of these models, the CPA and the NRHB equations of state and the emphasis is on the analysis of their predictive capabilities for a wide range of applications. We use the term predictive in two situations: (i) with no use of binary interaction parameters, and (ii) multicomponent calculations using binary interaction parameters based solely on binary data. It is shown that the CPA equation of state can satisfactorily predict CO2–water–glycols–alkanes VLE and water–MEG–aliphatic hydrocarbons LLE using interaction parameters obtained from the binary data alone. Moreover, it is demonstrated that the NRHB equation of state is a versatile tool which can be employed equally well to mixtures with pharmaceuticals and solvents, including mixed solvents, as well as phase equilibria in mixtures containing glycols. The importance of considering the solvation of CO2–water (in CPA) when the model is applied to multicomponent mixtures as well as of the multiple associations in heavy glycol–water mixtures (in NRHB) is investigated.
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.

General information
State: Published
Organisations: CERE – Center for Energy Resources Engineering, Department of Chemical and Biochemical
Engineering, Computer Aided Process Engineering Center, Center for Energy Resources Engineering
Authors: Yuan, H. (Intern), Sin, G. (Intern)
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Main Research Area: Technical/natural sciences

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Journal: Chemical Engineering Journal
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BFI (2017): BFI-level 2
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BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 6.34
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 5.68
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 4.92
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 4.59
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 3.92
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): CiteScore 3.96
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Web of Science (2008): Indexed yes
Web of Science (2007): Indexed yes
Web of Science (2005): Indexed yes
Web of Science (2003): Indexed yes
Upscaling of Two-Phase Immiscible Flows in Communicating Stratified Reservoirs

A semi-analytical method for upscaling two-phase immiscible flows in heterogeneous porous media is described. This method is developed for stratified reservoirs with perfect communication between layers (the case of vertical equilibrium), in a viscous dominant regime, where the effects of capillary forces and gravity may be neglected. The method is discussed on the example of its basic application: waterflooding in petroleum reservoirs. We apply asymptotic analysis to a system of two-dimensional (2D) mass conservation equations for incompressible fluids. For high anisotropy ratios, the pressure gradient in vertical direction may be set zero, which is the only assumption of our derivation. In this way, the 2D Buckley–Leverett problem may be reduced to a one-dimensional problem for a system of quasi-linear hyperbolic equations, of a number equal to the number of layers in the reservoir. They are solved numerically, based on an upstream finite difference algorithm. Self-similarity of the solution makes it possible to compute pseudofractional flow functions depending on the average saturation. The computer partial differential equation solver COMSOL is used for comparison of the complete 2D solutions with averaged 1D simulations. Cases of both discrete and continuous (log-normal) permeability distribution are studied. Generally, saturation profiles of the 1D model are only slightly different from the 2D simulation results. Recovery curves and fractional flow curves fit well. Calculations show that at a favorable mobility ratio (displaced to displacing phase) crossflow increases the recovery, while at an unfavorable mobility ratio, the effect is the opposite. Compared with the classical Hearn method, our method is more general and more precise, since it does not assume universal relative permeabilities and piston-like displacement, and it presumes non-zero exchange between layers. The method generalizes also the study of Yortsos (Transp Porous Media 18:107–129, 1995), taking into account in a more consistent way the interactions between the layers.
CO2 Flooding in Chalk Reservoirs

General information
State: Published
Organisations: CERE – Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, Department of Chemistry
Authors: Niu, B. (Intern), Shapiro, A. (Intern), Yan, W. (Intern), Stenby, E. H. (Intern)
Number of pages: 177
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Original language: English
Main Research Area: Technical/natural sciences

Multiphase Equilibrium in Systems with Production Chemicals

General information
State: Published
Chilled Ammonia Process for CO2 Capture

The chilled ammonia process absorbs the CO2 at low temperature (2–10°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 heat requirement. However, a scientific understanding of the processes is required. The thermodynamic 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°C and pressure up to 100 bars. The results show that solid phases consisting of ammonium carbonate and bicarbonate are formed in the absorber. The heat requirements in the absorber and in the desorber have been studied. The enthalpy calculations show that a heat requirement for the desorber lower than 2 GJ/ton CO2 can be reached.

General information

State: Published
Organisations: CERE – Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering
Authors: Darde, V. C. A. (Intern), Thomsen, K. (Intern), Well, W. J. V. (Ekstern), Stenby, E. H. (Intern)
Pages: 131-136
Publication date: Mar 2010
Main Research Area: Technical/natural sciences
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.
Advanced Waterflooding in Carbonate Reservoirs

General information
State: Published
Organisations: CERE – Center for Energy Ressources Engineering, Department of Chemical and Biochemical Engineering
Authors: Zahid, A. (Intern), Stenby, E. H. (Intern), Shapiro, A. (Intern)
Publication date: 2010
Event: Poster session presented at 11th International Symposium on Evaluation of Wettability and Its Effect on Oil Recovery, University of Calgary, Alberta, Canada, .
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 251918
Publication: Research - peer-review › Journal article – 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 pore 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)
Pages: 2473-2494
Publication date: 2010
Main Research Area: Technical/natural sciences

Publication information
Journal: Physica A: Statistical Mechanics and its Applications
Volume: 389
Issue number: 13
ISSN (Print): 0378-4371
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Monte Carlo simulation methods for determining fluid- and crystal-phase chemical potentials are used for the first time to calculate liquid water-methane hydrate-methane vapor phase equilibria from knowledge of atomistic interaction potentials alone. The water and methane molecules are modeled using the TIP4P/ice potential and a united-atom Lennard-Jones potential, respectively. The equilibrium calculation method for this system has three components, (i) thermodynamic integration from a supercritical ideal gas to obtain the fluid-phase chemical potentials, (ii) calculation of the chemical potential of the zero-occupancy hydrate system using thermodynamic integration from an Einstein crystal reference state, and (iii) thermodynamic integration to obtain the water and guest molecules' chemical potentials as a function of the hydrate occupancy. The three-phase equilibrium curve is calculated for pressures ranging from 20 to 500 bar and is shown to follow the Clapeyron behavior, in agreement with experiment; coexistence temperatures differ from the latter by 4-16 K in the pressure range studied. The enthalpy of dissociation extracted from the calculated P-T curve is within 2% of the experimental value at corresponding conditions. While computationally intensive, simulations such as these are
essential to map the thermodynamically stable conditions for hydrate systems.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering
Authors: Jensen, L. (Intern), Thomsen, K. (Intern), von Solms, N. (Intern), Wierzchowski, S. (Ekstern), Walsh, M. (Ekstern), Koh, C. (Ekstern), Sloan, E. (Ekstern), Wu, D. (Ekstern), Sum, A. (Ekstern)
Pages: 5775-5782
Publication date: 2010
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Physical Chemistry Part B: Condensed Matter, Materials, Surfaces, Interfaces & Biophysical
Volume: 114
Issue number: 17
ISSN (Print): 1520-6106
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
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
Scopus rating (2013): SJR 1.494 SNIP 1.2 CiteScore 3.53
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.92 SNIP 1.251 CiteScore 3.66
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.78 SNIP 1.226 CiteScore 3.62
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.849 SNIP 1.214
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 2.232 SNIP 1.349
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 2.543 SNIP 1.381
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 2.346 SNIP 1.282
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 2.369 SNIP 1.415
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 2.275 SNIP 1.474
Web of Science (2005): Indexed yes
Comparison of activity coefficient models for electrolyte systems

Three activity coefficient models for electrolyte solutions were evaluated and compared. The activity coefficient models are: The electrolyte NRTL model (ElecNRTL) by Aspentech, the mixed solvent electrolyte model (MSE) by OLI Systems Inc., and the Extended UNIQUAC model from the Technical University of Denmark (DTU). Test systems containing a single salt (NaCl), multiple salts, and mixed solvent aqueous electrolyte solutions were chosen. The performance of the activity coefficient models were compared regarding the accuracy of solid-liquid and vapor-liquid equilibrium calculations for the test systems.

General information
State: Published
Organisations: CERE – Center for Energy Ressources Engineering, Department of Chemical and Biochemical Engineering, Haldor Topsoe AS, Akzo Nobel Functional Chemicals AB, Shell Global Solutions (Malaysia), Sdn Bhd
Compositional Simulation of In-Situ Combustion EOR: A Study of Process Characteristics

General information
State: Published
Organisations: CERE – Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering
Authors: Jain, P. (Intern)
Publication date: 2010

Host publication information
Title of host publication: Proceedings from SPE Improved Oil Recovery Symposium
Main Research Area: Technical/natural sciences
Conference: SPE Improved Oil Recovery Symposium, Tulsa, Oklahoma, USA, 01/01/2010
Source: orbit
Source-ID: 274746
Publication: Research - peer-review › Article in proceedings – Annual report year: 2010

COMSOL Implementation for Two-Phase Immiscible Flows in Layered Reservoir

General information
State: Published
Organisations: CERE – Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering
Authors: Zhang, X. (Intern)
Publication date: 2010

Host publication information
Title of host publication: Proceedings from European COMSOL Conference
Main Research Area: Technical/natural sciences
Conference: European COMSOL Conference, Paris, France, 01/01/2010
Source: orbit
Source-ID: 274775
Publication: Research - peer-review › Article in proceedings – Annual report year: 2010

Design of a Eutectic Freeze Crystallization process for multicomponent waste water stream
Complex, hypersaline brines originating from the mining and extractive metallurgical industries have the potential to be treated using Eutectic Freeze Crystallization (EFC). Although EFC has been shown to be effective in separating a single salt and water, it has yet to be applied to the complex hypersaline brines that are typical of reverse osmosis retentates in South Africa. This paper focuses on the application of EFC for the purification of a typical brine containing high levels of sodium, chloride, sulphate and ammonia that cannot be achieved with other separation techniques. The presence of ammonia prevents the application of membrane technology to treat the brine, leaving only cooling or evaporation as other possible options. Evaporation produces a mixed salt that requires further treatment. Modelling tools were applied to describe the phase behaviour of the complex saline systems under different process conditions and were experimentally validated. The results showed that Eutectic Freeze Crystallization could be used to selectively recover the sodium as a sodium sulphate salt. The simulation tools were especially useful in the design and optimisation of the process.

General information
State: Published
Estimation of Migration and Diffusion Coefficients of GRINDSTED(R) SOFT-N-SAFE from PVC into Iso-octane

General information
State: Published
Organisations: CERE – Center for Energy Ressources Engineering, Department of Chemical and Biochemical Engineering
Authors: Lundsgaard, R. (Intern)
Publication date: 2010
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 266700
Publication: Research - peer-review › Journal article – Annual report year: 2010

Experimental investigation and molecular simulation of gas hydrates

General information
State: Published
Organisations: CERE – Center for Energy Ressources Engineering, Department of Chemical and Biochemical Engineering
Authors: Jensen, L. (Intern), von Solms, N. (Intern)
Number of pages: 196
Publication date: 2010

Publication information
Place of publication: Kgs. Lyngby, Denmark
Publisher: Technical University of Denmark (DTU)
ISBN (Print): 978-87-92481-29-0
Original language: English
Main Research Area: Technical/natural sciences
Electronic versions:
61379_PhD_Lars Jensen_WEB_.pdf
Source: orbit
Source-ID: 273737
Publication: Research › Ph.D. thesis – Annual report year: 2010

Extensive Comparison of Cubic Plus Association (CPA) and PC-SAFT Equations of State

General information
State: Published
Organisations: CERE – Center for Energy Ressources Engineering, Department of Chemical and Biochemical Engineering
Publication date: 2010
Event: Poster session presented at SAFT2010 : Special Symposium:20 years of the SAFT equation: Recent advantages and challenges, Barcelona, Spain.
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 274751
Publication: Research - peer-review › Poster – Annual report year: 2010

As a part of a series of reviews, a compilation of systems for which high-pressure phase-equilibrium data were published between 2000 and 2004 is given. Vapor-liquid equilibria, liquid-liquid equilibria, vapor-liquid-liquid equilibria, solid-liquid equilibria, solid-vapor equilibria, solid-vapor-liquid equilibria, critical points, the solubility of high-boiling substances in supercritical fluids, the solubility of gases in liquids and the solubility (sorption) of volatile components in polymers are included. For the systems investigated, the reference, the temperature and pressure range of the data, and the experimental method used for the measurements are given in 54 tables. Most of experimental data in the literature have been given for binary systems. Of the 1204 binary systems, 681 (57%) have carbon dioxide as one of the components. Information on 156 pure components, 451 ternary systems of which 267 (62%) contain carbon dioxide, 150 multicomponent and complex systems, and 129 systems with hydrates is given. Experimental methods for the investigation of high-pressure phase equilibria are classified and described. Work on the continuation of the review series is under way, covering the period between 2005 and 2008, and will be published in 2010. (C) 2009 Elsevier B.V. All rights reserved.
How to Model CO2 Capture

General information
State: Published
Organisations: CERE – Center for Energy Ressources Engineering, Department of Chemical and Biochemical Engineering
Improved Oil Recovery in Chalk: Wettability Alteration or Something Else?

General information
State: Published
Organisations: CERE – Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering
Authors: Zahid, A. (Intern), Stenby, E. H. (Intern), Shapiro, A. (Intern)
Publication date: 2010
Main Research Area: Technical/natural sciences

Publication information
Journal: SPE Journal
Volume: 131300
ISSN (Print): 1086-055X
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 0.95 SNIP 2.003 CiteScore 3.01
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
Industrial Requirements for Thermodynamic and Transport Properties

General information
State: Published
Organisations: CERE – Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering
Authors: Hemptine, J. D. (Ekstern), Hendriks, E. (Ekstern), Kontogeorgis, G. (Intern), Dohrn, R. (Ekstern), Economou, I. (Ekstern), Zilnik, L. (Ekstern), Vesovic, V. (Ekstern)
Publication date: 2010

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 274745
Publication: Research - peer-review › Journal article – Annual report year: 2010

Inhibition of Gas Hydrate Formation by Antifreeze Proteins

General information
State: Published
Organisations: CERE – Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering
Authors: Jensen, L. (Intern)
Publication date: 2010
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 274750
Publication: Research - peer-review › Poster – Annual report year: 2010

Inhibition of Gas Hydrate Formation by Low-Dosage, Environmentally Benign Inhibitors

General information
State: Published
Organisations: CERE – Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering
Authors: Jensen, L. (Intern)
Publication date: 2010

Host publication information
Title of host publication: Proceedings of the 2nd Annual Gas Processing Symposium
ISBN (Print): 978-0-444-53588-7
Main Research Area: Technical/natural sciences
Conference: 2nd Annual Gas Processing Symposium, Doha, Qatar, 11/01/2010 - 11/01/2010
Source: orbit
Source-ID: 274747
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 Ressources Engineering, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Jensen, L. (Intern), Ramløv, H. (Ekstern), Thomsen, K. (Intern), von Solms, N. (Intern)
Pages: 1486-1492
Publication date: 2010
Main Research Area: Technical/natural sciences

Publication information
Journal: Industrial & Engineering Chemistry Research
Volume: 49
Issue number: 4
ISSN (Print): 0888-5885
Ratings:
BFI (2018): BFI-level 2
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
Integrating chemical engineering fundamentals in the capstone process design project

All B.Eng. courses offered at the Technical University of Denmark (DTU) must now follow CDIO standards. The final “capstone” course in the B.Eng. education is Process Design, which for many years has been typical of chemical engineering curricula worldwide. The course at DTU typically has about 30 students. The B.Eng. education lasts for 3½ years (seven semesters), of which the 5th semester consists of practical training with a company and the final (7th) semester consists of a research project. The design course falls in the 6th semester, and is thus the last formal instruction that the students receive. The education is designed to provide students with the necessary tools to become productive in a company in a short time – so there is a strong industrial focus. Some students choose to continue with their studies and can then complete an M.Sc. after a further two years of study. The demands of the CDIO standards – especially standard 3 – Integrated Curriculum - means that the course projects must draw on competences provided in other subjects which the students are taking in parallel with Process Design – specifically Process Control and Reaction Engineering. In each semester of the B.Eng. education, one course is designated the “project” course, which should draw on material learned in parallel courses. In the 6th semester, Process Design is the project course. Process Control and Reaction Engineering are then incorporated into the final plant design project. Specifically, almost all chemical plants will incorporate one or more chemical reactors. In the initial stages of a process design, it is sufficient to express simply the reactor inputs and outputs. However in later stages, details about the reactor need to be specified. This is only possible using tools learned in the course Reaction Engineering. In order to incorporate reactor design into process design in a meaningful way, the teachers of the respective courses need to collaborate (Standard 9 – Enhancement of Faculty CDIO skills). The students also see that different components of the chemical engineering curriculum relate to each other. Similarly, in process design, steady state is always assumed for processes (i.e. production of a given chemical occurs at a constant rate, temperature, pressure and composition; feeds enter the plant at constant rates, etc.). However, in practice, chemical plants need to be carefully controlled to operate at a specified set of steady-state conditions. This is the science of Process Control and the students are asked to apply what they have learned here in order to show how to control the operation of the plant they have designed. The key difference from typical (earlier) process design courses is that the interaction between the courses is formalized, requiring (amongst other things) increased, broader teacher competence and communication between teachers across different disciplines, thereby also tying in with Standard 9 – Enhancement of Faculty CDIO skills.
From a CDIO perspective, Process Design provides an opportunity for a comprehensive implementation of CDIO principles in a single course. Already the traditional chemical engineering "capstone" design course has for decades embodied many of the essential features of CDIO (for example the focus on group work, development of interpersonal skills, the open-ended nature of design problems, etc.).

**General information**

State: Published
Organisations: CERE – Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, CHEC Research Centre, Computer Aided Process Engineering Center
Authors: von Solms, N. (Intern), Woodley, J. (Intern), Johnsson, J. E. (Intern), Abildskov, J. (Intern)
Publication date: 2010

**Host publication information**

Title of host publication: Proceedings of CDIO conference
Main Research Area: Technical/natural sciences
Conference: CDIO conference, Montreal, Canada, 01/01/2010
Enhancement of Faculty CDIO skills, Integrated Curriculum, Process Design, Capstone Project
Electronic versions:
PEC10-50.pdf
Links:
http://www.cdio.org/knowledge-library/documents/integrating-chemical-engineering-fundamentals-capstone-process-design-pr
Source: orbit
Source-ID: 268739
Publication: Research - peer-review › Article in proceedings – Annual report year: 2010

**Intramolecular Association within the SAFT Framework**

**General information**

State: Published
Organisations: CERE – Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering
Authors: Avlund, A. S. (Intern)
Publication date: 2010

**Publication information**

Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 274786
Publication: Research › Sound/Visual production (digital) – Annual report year: 2010

**Intramolecular Association within the SAFT Framework**

**General information**

State: Published
Organisations: CERE – Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering
Authors: Avlund, A. S. (Intern)
Publication date: 2010
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 274738
Publication: Research - peer-review › Poster – Annual report year: 2010

**Intramolecular Association within the SAFT Framework**

**General information**

State: Published
Organisations: CERE – Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering
Microbial Enhanced Oil Recovery: 3D Simulation with Gravity Effects

Microbial enhanced oil recovery (MEOR) utilizes the activity of microorganisms, where microorganisms simultaneously grow in a reservoir and convert substrate into recovery enhancing products (usually, surfactants). In order to predict the performance of a MEOR process, a simulation tool is required, with all the relevant physical processes included.

We have developed a mathematical model describing the process of MEOR, where reactive transport is combined with a simple compositional approach. The model describes the displacement of oil by water containing bacteria, substrate, and the produced metabolite, surfactant. The metabolite is allowed to partition between the oil and water phases according to a distribution coefficient. Production of surfactant decreases the oil/water interfacial tension, reduces the residual oil saturation, and provides additional oil recovery.

In this work, we have implemented our MEOR model into a compositional streamline simulator based on the standard IMPEC framework (implicit pressure, explicit composition) to decouple flow and reactive transport. The reaction and transport processes are solved simultaneously along each streamline. Gravity effects are implemented using an operator splitting technique. To the best of our knowledge, this has resulted in the first full 3D MEOR streamline simulator. For verification purposes, we compare results from our streamline MEOR simulator to those of a conventional finite difference approach for 1D and 2D displacement calculations.

We investigate the benefit of MEOR relative to water flooding, comparing the processes in multiple dimensions. The results of our simulations demonstrate that the oil recovery from MEOR processes in relation to water flooding is markedly increased, and the high recovery is achieved much faster. In addition, the compositional streamline simulator is applied to study both microscopic and macroscopic displacement efficiency of MEOR.
In this project, a generic model has been set up to include the two main mechanisms in the microbial enhanced oil recovery (MEOR) process; reduction of the interfacial tension (IFT) due to surfactant production, and microscopic fluid diversion as a part of the overall fluid diversion mechanism due to formation of biofilm. The construction of a one-dimensional simulator enables us to investigate how the different mechanisms and the combination of these influence the displacement processes, the saturation profiles and thus the oil recovery curves. The reactive transport model describes convection, bacterial growth, substrate consumption, and surfactant production in one dimension. The system comprises oil, water, bacteria, substrate, and surfactant. There are two flowing phases: Water and oil. We introduce the partition of surfactant between these two phases determined by a partitioning constant. Another effect is attachment of the bacteria to the pore walls and formation of biofilm. It leads to reduction of porosity and, under some assumptions, to increase the fraction of oil in the flow. Surfactant is our key component in order to reduce IFT. The surfactant concentration in the water phase must reach a certain concentration threshold, before it can reduce the interfacial tension and, thus, the residual oil saturation. The relative permeabilities depend on the water phase concentration, so when surfactant is moved into the oil phase, the effect from the surfactant on the oil production is reduced. Therefore, the transfer part of the surfactant to oil phase is equivalent to its “disappearance”. The oil phase captures the surfactant, but it may as well be adsorbed to the pore walls in the oil phase. We have looked into three methods how to translate the IFT reduction into changes of the relative permeabilities. Overall, these methods produce similar results. Separate investigations of the surfactant effect have been performed through exemplifying simulation cases, where no biofilm is formed. The water phase saturation profiles are found to contain a waterfront initially following the saturation profile for pure waterflooding. At the oil mobilization point – where the surfactant effect starts to take place – a sufficient surfactant concentration has been built up in order to mobilize the residual oil. A second waterfront is produced, and an oil bank is created. The recovery curve consists of several parts. Initially, the recovery curve follows pure waterflooding recovery until breakthrough of the oil bank. The next part of the recovery curve continues until breakthrough of the second waterfront. The incline is still relatively steep due to a low water cut. In the last part, the curve levels off. Partitioning of surfactant between the oil and water phase is a novel effect in the context of microbial enhanced oil recovery. The partitioning coefficient determines the time lag before the surfactant effect can be seen. The surfactant partitioning does not change final recovery, but a smaller partitioning coefficient gives a larger time lag before the same maximum recovery is reached. However, if too little surfactant stays in the water phase, we cannot obtain the surfactant effect. The final recovery depends on the distance from the inlet to the oil mobilization point. Additionally, it depends on, how much the surfactant-induced IFT reduction lowers the residual oil. The surfactant effect position is sensitive to changes in growth rate, and injection concentrations of bacteria and substrate, which then determine the final recovery. Variations in growth rate and injection concentration also affect the time lag until mobilization of residual oil occurs. Additionally, the final recovery depends on, how much the surfactant-induced interfacial tension reduction lowers the residual oil saturation. The effects of the efficiency of surfactants are also investigated. A super efficient surfactant produces an incremental recovery recovery around 40 % OOIP over that of waterflooding. Application of the less efficient – and probably more realistic -- surfactant results in an incremental oil recovery of 9 % OOIP, but it is still considered a significant improvement. The bacteria may adhere to the pore walls and form a biofilm phase. The bacteria distribution between the water and biofilm phase is modeled by the Langmuir expression, which depends on the bacteria concentration in the water phase. The surface available for adsorption is scaled by the water saturation, as bacteria only adsorb from the water phase. The biofilm formation implies that the concentration of bacteria near the inlet increases. In combination with surfactant production, the biofilm results in a higher surfactant concentration in the initial part of the reservoir. The oil that is initially bypassed in connection with the surfactant effect, can be recovered as formation of biofilm shortens the distance from the inlet to the point of oil mobilization. The effect of biofilm formation on the displacement profiles and on the recovery is studied in the present work. Formation of biofilm also leads to porosity reduction, which is coupled to modification of permeability. This promotes the fluid diversion mechanism. A contribution to fluid diversion mechanism is microscopic fluid diversion, which is possible to investigate in a one-dimensional system. The relative permeability for water is modified according to our modified version of the Kozeny-Carman equation. Bacteria only influence the water and biofilm phases directly, so the oil phase remains the same. We have assessed the effect from biofilm formation together with microscopic fluid diversion. When sufficient amount of surfactant is produced in the water phase, the effect from surfactant generates a larger contribution to recovery compared to microscopic fluid diversion. To study the MEOR performance in multiple dimensions, the one-dimensional model with the surfactant effect alone has been implemented into existing simulators; a streamline simulator and a finite difference simulator. In the streamline simulator, the effect of gravity is introduced using an operator splitting technique. The gravity effect stabilizes oil displacement causing markedly improvement of the oil recovery, when the oil density becomes relatively low. The general characteristics found for MEOR in one-dimensional simulations are also demonstrated both in two and three dimensions. Overall, this MEOR process conducted in a heterogeneous reservoir also produces more oil compared to waterflooding, when the simulations are run in multiple dimensions. The work presented in this thesis has resulted in two publications so far.
Modeling Non-Fickian Transport and Hyperexponential Deposition for Deep Bed Filtration

An integral model of the deep bed filtration process has been developed. It incorporates pore and particle size distributions, as well as the particle residence time distribution in the framework of the continuous time random walk theory. Numerical modeling is carried out to study the factors influencing breakthrough curves and deposition profiles for the deep bed filtration systems. Results are compared with a large set of experimental observations. Our findings show that highly dispersed breakthrough curves, e.g. those with early arrivals and large ending tails, correspond to large dispersion coefficients. For such cases the elliptic equation excels the advection dispersion equation in both fitting breakthrough curves and predicting deposition profiles related to natural or highly heterogeneous porous media. The deposition hyperexponentiality can be caused by the following three mechanisms: particle population in connection with the distribution of the filtration coefficients, heterogeneity in connection with non-Fickian transport, and heterogeneity in connection with the spatial distribution of the filtration coefficients. The influence and interaction of all three mechanisms have been analyzed in numerical computations and by comparison to several sets of experimental data.
Modeling of carbon dioxide absorption by aqueous ammonia solutions using the Extended UNIQUAC model

An upgraded version of the Extended UNIQUAC thermodynamic model for the carbon dioxide-ammonia-water system has been developed, based on the original version proposed by Thomsen and Rasmussen. The original model was valid in the temperature range 0-110°C, the pressure range 0-10 MPa and the concentration range up to 80 molal ammonia. In this work, the validity of this model was extended up to 150°C and the accuracy improved by increasing the number of experimental data points from 2000 to more than 3500. These experimental data consisting of vapor-liquid equilibrium data in various concentration ranges, enthalpy change from partial evaporation measurements, speciation data, heat capacity, enthalpy of solution and enthalpy of dilution data have been used to refit 43 model parameters and standard state properties. Henry’s law constant correlations have been used for extrapolating standard state properties of carbon dioxide and ammonia to supercritical conditions.

General information
State: Published
Organisations: CERE – Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, DONG Energy A/S
Authors: Darde, V. C. A. (Intern), van Well, W. J. M. (Ekstern), Stenby, E. H. (Intern), Thomsen, K. (Intern)
Pages: 12663-12674
Publication date: 2010
Main Research Area: Technical/natural sciences

Publication information
Journal: Industrial & Engineering Chemistry Research
Volume: 49
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Ratings:
BFI (2018): BFI-level 2
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
Modeling Phase Equilibria for Acid Gas Mixtures Using the CPA Equation of State. I. Mixtures with H2S

The Cubic-Plus-Association (CPA) equation of state is applied to a large variety of mixtures containing H2S, which are of interest in the oil and gas industry. Binary H2S mixtures with alkanes, CO2, water, methanol, and glycols are first considered. The interactions of H2S with polar compounds (water, methanol, and glycols) are modeled assuming presence or not of cross-association interactions. Such interactions are accounted for using either a combining rule or a cross-solvation energy obtained from spectroscopic data. Using the parameters obtained from the binary systems, one
ternary and three quaternary mixtures are considered. It is shown that overall excellent correlation for binary, mixtures and satisfactory prediction results for multicomponent systems are obtained. There are significant differences between the various modeling approaches and the best results are obtained when cross association is explicitly accounted for, especially using the cross-association energy from independent experimental studies rather than from combining rules.

**General information**

State: Published
Organisations: CERE – Center for Energy Ressources Engineering, Department of Chemical and Biochemical Engineering
Authors: Tsivintzelis, I. (Intern), Kontogeorgis, G. (Intern), Michelsen, M. L. (Intern), Stenby, E. H. (Intern)
Pages: 2965-2982
Publication date: 2010
Main Research Area: Technical/natural sciences

**Publication information**

Journal: A I Ch E Journal
Volume: 56
Issue number: 11
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Ratings:
- BFI (2018): BFI-level 2
- BFI (2017): BFI-level 2
- Web of Science (2017): Indexed Yes
- BFI (2016): BFI-level 2
- Web of Science (2016): Indexed yes
- Scopus rating (2016): CiteScore 3.11 SJR 1.034 SNIP 1.268
- Web of Science (2015): 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
- 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
- Scopus rating (2007): SJR 1.256 SNIP 1.341
- Web of Science (2007): Indexed yes
- Scopus rating (2006): SJR 1.483 SNIP 1.612
- Web of Science (2006): Indexed yes
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.

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)
Pages: 185-188
Publication date: 2010

Host publication information
Title of host publication: Graduate Schools Yearbook 2010
Publisher: Technical University of Denmark, Department of Chemical Engineering
ISBN (Print): 978-87-92481-36-8
Main Research Area: Technical/natural sciences
Electronic versions: KTyearbook_2010HY.pdf
Source: orbit
Source-ID: 277534
Publication: Research › Book chapter – Annual report year: 2011

Modeling the Phase Behavior of Mixtures used in Oxidation of Alcohols in Supercritical CO2

General information
State: E-pub ahead of print
Organisations: CERE – Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering
Authors: Tsivintzelis, I. (Intern), Beier, M. (Ekstern), Grunwaldt, J. (Ekstern), Kontogeorgis, G. (Intern)
Publication date: 2010
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 274772
Publication: Research - peer-review › Poster – Annual report year: 2010
Modelling of Partition Coefficients of Additives in Polymer/solvent Systems by Free Energy Calculations

General information
State: Published
Organisations: CERE – Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering
Authors: Lundsgaard, R. (Intern)
Publication date: 2010
Event: Poster session presented at Molecular Modelling and Simulation for Industrial Applications: Physico-Chemical Properties and Processes, Wurzburg, Germany.
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 274755
Publication: Research - peer-review › Poster – Annual report year: 2010

Modelling of Partition Coefficients of Additives in Polymer/solvent Systems by Free Energy Calculations

General information
State: Published
Organisations: CERE – Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering
Authors: Lundsgaard, R. (Intern)
Publication date: 2010
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 274756
Publication: Research - peer-review › Poster – Annual report year: 2010

Modelling of Partition Coefficients of Additives in Polymer/solvent Systems by Free Energy Calculations

General information
State: Published
Organisations: CERE – Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering
Authors: Lundsgaard, R. (Intern)
Publication date: 2010
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 274758
Publication: Research - peer-review › Poster – Annual report year: 2010

Modelling the Phase Equilibria with CPA using the Homomorph Approach

General information
State: Published
Organisations: CERE – Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering
Authors: Martin, B. (Ekstern), Tsivintzelis, I. (Intern), Kontogeorgis, G. (Intern)
Publication date: 2010
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 274740
Publication: Research - peer-review › Poster – Annual report year: 2010

Monte-Carlo Simulations of the Liquid Water-Hydrate-Methane Vapor Phase Equilibria
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.

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 at e used Methanol-alkane vapor-liquid equilibrium (VLE) and liquid-liquid equilibrium (LLE) data. 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
Phase Equilibria of Mixtures Containing Organic Sulfur Species (OSS) and Water/Hydrocarbons: VLE Measurements and Modeling Using the Cubic-Plus-Association Equation of State

We report new vapor–liquid equilibrium (VLE) data for dimethyl sulfide (DMS) in pure water, performed at three temperatures (303, 330, and 362 K) in the 1–8 MPa pressure range. The total system pressure was maintained introducing CH4. The inlet mole fraction of DMS was the same in all experiments, around $1.5 \times 10^{-3}$ in the liquid phase. A "static-analytic" method was used for performing all of the measurements. The objective is to provide experimental VLE data for the dimethyl sulfide + CH4 + water system, for which no data are available in the open literature. These data will allow industry to model sulfur emissions. The new VLE data as well as the VLE data of some binary systems from the literature containing organic sulfur species + hydrocarbon, organic sulfur species + water, and some ternary systems containing organic sulfur species in hydrocarbons and water have been modeled successfully with the cubic-plus-association (CPA) equation of state. Useful remarks are presented about the application of Henry’s constant values to estimate binary interaction parameters of the CPA EoS for the description of whole vapor–liquid equilibria. The results using CPA EoS show that the cross association interactions in the methyl mercaptan + water system and ethyl mercaptan + water system should be considered. In aqueous mixtures of higher mercaptans, the consideration of such interactions does not improve the calculations, indicating that they are rather weak.

General information
State: Published
Organisations: CERE – Center for Energy Ressources Engineering, Department of Chemical and Biochemical Engineering, Novo Nordisk A/S, MINES ParisTech
Authors: Awan, J. (Intern), Tsivintzelis, I. (Intern), Breil, M. (Ekstern), Coquelet, C. (Ekstern), Richon, D. (Ekstern), Kontogeorgis, G. (Intern)
Pages: 12718-12725
Publication date: 2010
Main Research Area: Technical/natural sciences

Publication information
Journal: Industrial & Engineering Chemistry Research
Volume: 49
Issue number: 210
ISSN (Print): 0888-5885
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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
Phase Equilibrium with Surfactant Model System at Elevated Pressures

General information
State: Published
Organisations: CERE – Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering
Authors: Sandersen, S. B. (Intern)
Publication date: 2010
Post-Combustion Capture of CO2 from Fossil Fueled Power Plants

General information
State: Published
Organisations: CERE – Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering
Authors: Faramarzi, L. (Intern), Kontogeorgis, G. (Intern), Thomsen, K. (Intern), Stenby, E. H. (Intern)
Number of pages: 96
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, 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

Publication information
Journal: Carbohydrate Polymers
Volume: 79
Issue number: 3
ISSN (Print): 0144-8617
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 5.15 SJR 1.404 SNIP 1.745
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
PVT Modeling of Reservoir Fluids using PC-SAFT EoS and Soave-BWR EOS

General information
State: Published
Organisations: CERE – Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering
Authors: Yan, W. (Intern), Stenby, E. H. (Intern)
Publication date: 2010

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Recent Applications of the CPA Equations of State

General information
State: Published
Organisations: CERE – Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering
Authors: Tsivintzelis, I. (Intern), Kontogeorgis, G. (Intern), Michelsen, M. L. (Intern), Stenby, E. H. (Intern)
Publication date: 2010
Event: Poster session presented at SAFT2010 : Special Symposium: 20 years of the SAFT equation: Recent advantages and challenges, Barcelona, Spain.
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 274773
Publication: Research › Poster – Annual report year: 2010

Recovery of Phosphate from Waste: Thermodynamic Modeling of Phosphate Systems

General information
State: Published
Organisations: CERE – Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering
Authors: Thomsen, K. (Intern)
Publication date: 2010
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 274769
Publication: Research › Poster – 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.
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<tr>
<td>Organisations: CERE – Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering, Technical University of Denmark</td>
</tr>
<tr>
<td>Authors: von Solms, N. (Intern), Kristensen, J. (Ekstern)</td>
</tr>
<tr>
<td>Pages: 19-25</td>
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<td>Publication date: 2010</td>
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<tr>
<td>Journal: International Journal of Refrigeration</td>
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<tr>
<td>Volume: 33</td>
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<td>Issue number: 1</td>
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<td>BFI (2009): BFI-level 1</td>
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<td>Web of Science (2009): Indexed yes</td>
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<td>Scopus rating (2007): SJR 0.841 SNIP 1.646</td>
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<td>Scopus rating (2005): SJR 1.409 SNIP 1.718</td>
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<td>Web of Science (2005): Indexed yes</td>
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<td>Scopus rating (2004): SJR 1.193 SNIP 1.933</td>
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<td>Scopus rating (2001): SJR 1.775 SNIP 1.86</td>
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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 Ressources 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
Publication date: 2010
Main Research Area: Technical/natural sciences

Publication information
Journal: Corrosion Engineering, Science and Technology
Volume: 45
Issue number: 2
ISSN (Print): 1478-422X
Ratings:
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BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 0.382 SNIP 0.588 CiteScore 0.86
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
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.333 SNIP 0.63
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.396 SNIP 0.786
Web of Science (2009): Indexed yes
Solid–liquid equilibria for binary and ternary systems with the Cubic-Plus-Association (CPA) equation of state
A systematic investigation of the CPA model's performance within solid-liquid equilibria (SLE) in binary mixtures (methane + ethane, methane + heptane, methane + benzene, methane + CO2, ethane + heptane, ethane + CO2, 1-propanol + 1,4-dioxane, ethanol + water, 2-propanol + water) is presented. The results from the binary mixtures are used to predict SLE behaviour in ternary mixtures (methane + ethane + heptane, methane + ethane + CO2). Our results are compared with experimental data found in the literature.

General information
State: Published
Organisations: CERE – Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering
Authors: Fettouhi, A. (Intern), Thomsen, K. (Intern)
Pages: 121-129
Publication date: 2010
Main Research Area: Technical/natural sciences

Publication information
Journal: Fluid Phase Equilibria
Volume: 293
Issue number: 2
ISSN (Print): 0378-3812
Ratings:
BFI (2018): BFI-level 2
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
Solid-Liquid Equilibria for Many-component Mixtures Using Cubic-Plus-Association (CPA) equation of state

In the creation of liquefied natural gas the formation of solids play a substantial role, hence detailed knowledge is needed about solid-liquid equilibria (SLE). In this abstract we shortly summarize the work we have carried out at CERE over the past year with SLE for many-component mixtures using the Cubic-Plus-Association (CPA) equation of state. Components used in this work are highly relevant to the oil and gas industry and include light and heavy hydrocarbons, alcohols, water and carbon dioxide.

General information
State: Published
Organisations: CERE – Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering
Authors: Fettouhi, A. (Intern), Thomsen, K. (Intern)
Pages: 136-137
Publication date: 2010
Tertiary Carbon Dioxide Flooding of Low Permeable Chalk with In-Situ Saturation Determination using X-Ray Computed Tomography

General information
State: Published
Organisations: CERE – Center for Energy Ressources Engineering, Department of Chemical and Biochemical Engineering
Authors: Niu, B. (Intern), Yan, W. (Intern), Shapiro, A. (Intern), Stenby, E. H. (Intern)
Publication date: 2010
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 274762
Publication: Research - peer-review › Poster – Annual report year: 2010

The Cubic Plus Association (CPA) Equation of State: What have we learnt in 15 years and future challenges

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CERE – Center for Energy Ressources Engineering
Authors: Kontogeorgis, G. (Intern), Tsivintzelis, I. (Intern), Michelsen, M. L. (Intern), Breil, M. (Ekstern), Stenby, E. H. (Intern)
Publication date: 2010

The Influence of CO2 Solubility in Brine on Simulation of CO2 Injection into Water Flooded Reservoir and CO2 WAG

Injection of CO2 into depleted oil reservoirs is not only a traditional way to enhance oil recovery but also a relatively cheaper way to sequester CO2 underground since the increased oil production can offset some sequestration cost. CO2 injection process is often applied to water flooded reservoirs and in many situations alternating injection of water and CO2 is required to stabilize the injection front. Both scenarios involve a large amount of water, making CO2 solubility in brine, which is around ten times higher than methane solubility, a non-negligible factor in the relevant reservoir simulations. In our previous study, a 1-D slitmube simulator, which rigorously accounts for both CO2 solubility in brine and water content in hydrocarbon phases using the Peng-Robinson EoS modified by Soreide and Whitson, has been used to investigate the influence of CO2 solubility on the simulation of continuous CO2 flooding with uniform initial water saturation. As a follow-up of the previous study, this study extends the investigation to two more realistic scenarios (1) CO2 injection into water flooded reservoir and (2) water-alternating-gas (WAG) injection with CO2 as the injection gas. A series of 1-D simulations were made for seven oil samples within a wide range of temperature, pressure and salinity. The results were analyzed in terms of the change in oil recovery due to different phase equilibrium descriptions, the delay in breakthrough and the CO2 lost to the aqueous phase. The influence of different factors, including temperature, pressure, salinity, water injection pore volume, WAG ratio and CO2 slug size, on the simulation results was also discussed. In addition, the results for CO2 injection into water flooded reservoirs were also compared with those from the previous study.

General information
State: Published
Organisations: CERE – Center for Energy Ressources Engineering, Department of Chemical and Biochemical Engineering
Authors: Yan, W. (Intern), Stenby, E. H. (Intern)
PAGES: 131094
Thermodynamic Applications in Petroleum, Energy, Material/Chemical and Biochemical Industries

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering
Authors: Kontogeorgis, G. (Intern)
Publication date: 2010
Event: Paper presented at University of Porto, Portugal.
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 274754
Publication: Research - peer-review › Conference abstract in proceedings – Annual report year: 2010

Thermodynamic Modeling of Sour Gas Cleaning Process

General information
State: Published
Organisations: CERE – Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering
Authors: Sadegh, N. (Intern)
Publication date: 2010

Host publication information
Title of host publication: Proceedings of the 21st IUPAC International Conference on Chemical Thermodynamics
Main Research Area: Technical/natural sciences
Conference: 21st IUPAC International Conference on Chemical Thermodynamics, Ibaraki, Japan, 01/08/2010 - 01/08/2010
Source: orbit
Source-ID: 275098
Publication: Research - peer-review › Conference abstract in proceedings – Annual report year: 2010

Thermodynamic Modeling of Sour Gas Cleaning Process

General information
State: Published
Organisations: CERE – Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering
Authors: Sadegh, N. (Intern)
Publication date: 2010

Host publication information
Title of host publication: Proceedings from SPE Conference STC-2010
Main Research Area: Technical/natural sciences
Conference: SPE Conference STC-2010, Germany, 01/01/2010
Thermodynamic Models for Industrial Applications: From Classical and Advanced Mixing Rules to Association Theories

General information
State: Published
Organisations: CERE – Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering
Authors: Kontogeorgis, G. (Intern), Folas, G. (Ekstern)
Number of pages: 710
Publication date: 2010

The Stability of Methane Hydrate from Molecular Simulation

General information
State: Published
Organisations: CERE – Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering
Authors: Jensen, L. (Intern)
Publication date: 2010
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 274749
Publication: Research - peer-review › Poster – Annual report year: 2010

Towards Predictive Association Theories

General information
State: E-pub ahead of print
Organisations: CERE – Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering
Authors: Kontogeorgis, G. (Intern), Tsivintzelis, I. (Intern), Folas, G. (Ekstern), Michelsen, M. L. (Intern), Stenby, E. H. (Intern)
Publication date: 2010

Host publication information
Title of host publication: Proceedings from the 12th International Conference on Properties and Phase Equilibria for Product and Process Design - digital edition
Main Research Area: Technical/natural sciences
Conference: 12th International Conference on Properties and Phase Equilibria for Product and Process Design, Suzhou, Jiangsu, China, 16/05/2010 - 16/05/2010
Source: orbit
Source-ID: 274753
Publication: Research - peer-review › Article in proceedings – Annual report year: 2010

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.

General information
State: Published
Organisations: CERE – Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering
Authors: Yuan, H. (Intern), Shapiro, A. (Intern), Stenby, E. H. (Intern)
Publication date: 2010
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 263787
Publication: Research › Poster – Annual report year: 2010

Tuning the catalytic Activity in the Selective Aerobic Alcohol Oxidation in Supercritical CO2 by Modeling the Phase Behavior

General information
State: Published
Organisations: CHEC Research Centre, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering
Authors: Beier, M. J. (Intern), Tsivintzelis, I. (Intern), Kontogeorgis, G. (Intern), Grunwaldt, J. (Intern)
Number of pages: 2
Publication date: 2010
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 266209
Publication: Research › Conference abstract for conference – Annual report year: 2010

Upscaling of Waterflooding in Porous Media

General information
State: Published
Organisations: CERE – Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering
Authors: Zhang, X. (Intern)
Publication date: 2010

Host publication information
Title of host publication: Proceedings from 12th European Conference on the Mathematics of Oil Recovery
Main Research Area: Technical/natural sciences
Conference: 12th European Conference on the Mathematics of Oil Recovery, Oxford, United Kingdom, 01/01/2010
Source: orbit
Source-ID: 274774
Publication: Research - peer-review › Article in proceedings – Annual report year: 2010

Use of Monomer Fraction Data in the Parametrization of Association Theories

Association theories such as the CPA (cubic-plus-association), NRHB (non-random hydrogen bonding) equations of state and the various variants of SAFT (statistical associating fluid theory) have been extensively applied to phase equilibrium calculations. Such models can also be used for estimating the monomer fraction of hydrogen bonding compounds and their mixtures. Monomer fraction data are obtained from spectroscopic measurements and they are available for a few compounds such as pure water and alcohols as well as for some alcohol–alkane and similar mixtures. These data are useful for an understanding of the capabilities and limitations of association models. The purpose of this work is two-fold: (i) to compare the performance of three models, CPA, NRHB and sPC-SAFT, in predicting the monomer fraction of water, alcohols and mixtures of alcohol-inert compounds and (ii) to investigate whether "improved" model parameters can be obtained if monomer fraction data are included in the parameter estimation together with vapor pressures and liquid densities. The expression "improved" implies parameters which can represent several pure compound properties as well as monomer fraction data for pure compounds and mixtures. The accuracy of experimental monomer fraction data is discussed, as well as the role of monomer fraction data in clarifying which association scheme should be used in these equations of state. The results reveal that the investigated association models (CPA, sPC-SAFT and NRHB) can predict,
at least qualitatively correct, monomer fractions of associating compounds and mixtures. Only, small differences are observed between the models. In addition, it has been shown that, using a suitable association scheme, a single set of parameters can describe satisfactorily vapor pressures, liquid densities and monomer fractions of water and alcohols. The 4C scheme is the best choice for water, while for methanol there is small difference between the 2B and 3B association schemes.
Vapor-Liquid Equilibrium Measurements and Modeling of the Propyl Mercaptan plus Methane plus Water System

In this work, vapor−liquid equilibrium (VLE) measurements of propyl mercaptan (PM) in pure water were performed at three different temperatures, (303, 323, and 365) K, with a pressure variation from (1 to 8) MPa. The total system pressure was maintained by CH4. The inlet mole fraction of propyl mercaptan in all experiments was the same, around 4.5·10−4 in the liquid phase. The objective was to provide experimental VLE data points of the propyl mercaptan + methane + water system for modeling since there is a lack of available data. These data will allow the industrial modeling of sulfur emission. The thermodynamic model used for the description of VLE is the extended UNIQUAC model. The model parameters are valid in the temperature range similar to the measured data and a pressure range up to 8 MPa.

General information
State: Published
Organisations: CERE – Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, MINES ParisTech
Authors: Awan, J. (Intern), Thomsen, K. (Intern), Coquelet, C. (Ekstern), Fosbøl, P. L. (Intern), Richon, D. (Ekstern)
Pages: 842-846
Publication date: 2010
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Chemical and Engineering Data
Volume: 55
Issue number: 2
ISSN (Print): 0021-9568
Ratings:
BFI (2018): BFI-level 2
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
Electrolyte Solutions: Thermodynamics, Crystallization, Separation methods

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering
Authors: Thomsen, K. (Intern)
Number of pages: 111
Publication date: 2009

Publication information
Capture and Storage Projects at IVC-SEP

General information
State: Published
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:
DTUEnergy_IVCPoster5_2_.pdf
Source: orbit
Source-ID: 232201
Publication: Research - peer-review › Poster – Annual report year: 2008

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
Host publication information
Title of host publication: Encyclopedia of Surface and Colloid Science
Place of publication: New York
Publisher: C R C Press LLC
Edition: Second
ISBN (Print): 9780849396151
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 191858
Publication: Research - peer-review › Book chapter – Annual report year: 2006

Modeling of Phase Equilibria for Paint-Related Polymer 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, CERE – Center for Energy Resources Engineering
Authors: Kouskoumvekaki, I. (Intern), Kontogeorgis, G. (Intern), Michelsen, M. L. (Intern)
Number of pages: 146
Publication date: Apr 2004
Publication information
Original language: English
Main Research Area: Technical/natural sciences
Electronic versions:
Source: orbit
**Thermodynamic Modelling of Surfactant Solutions**

**General information**
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering
Authors: Cheng, H. (Intern), Stenby, E. H. (Intern), Kontogeorgis, G. (Intern)
Publication date: Mar 2004

**Publication information**
Original language: English
Main Research Area: Technical/natural sciences
Electronic versions:
hongyuanCheng.pdf
Source: orbit
Source-ID: 192191
Publication: Research › Ph.D. thesis – Annual report year: 2004

**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
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
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
Modelling of Phase Equilibria Containing Associating Fluids

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CERE – Center for Energy Ressources Engineering
Authors: Derawi, S. (Intern), Stenby, E. H. (Intern), Kontogeorgis, G. (Intern)
Publication date: Feb 2003

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 209351
Publication: Research › Ph.D. thesis – Annual report year: 2003

Application of the CPA equation of state to industrially important systems

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CERE – Center for Energy Ressources Engineering
Application of the CPA Equation of State to Industrially Important Systems

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering
Authors: Derawi, S. (Intern), Folas, G. (Extern), Michelsen, M. L. (Intern), Stenby, E. H. (Intern), Kontogeorgis, G. (Intern)
Publication date: 2003
Event: Abstract from 15 Years of the SAFT Equation, Barcelona, Spain.
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 41318
Publication: Research › Conference abstract for conference – Annual report year: 2003

Applications of Association Models to Problems of the Oil, Chemical and Polymer Industries

General information
State: Published
Organisations: CERE – Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, Center for Biological Sequence Analysis, Department of Systems Biology, Center for Energy Resources Engineering
Pages: 93-96
Publication date: 2003

Host publication information
Title of host publication: Proceedings of the 20th European Symposium on Applied Thermodynamics
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: 209319
Publication: Research › Conference abstract in proceedings – Annual report year: 2003

Black Oil Streamline Simulator with Capillary Effects

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering
Authors: Berenblyum, R. (Intern), Shapiro, A. (Intern), Jessen, K. (Intern), Stenby, E. H. (Intern), Orr Jr., F. (Extern)
Publication date: 2003

Host publication information
Title of host publication: Proceedings of the Annual workshop of the IEA Collaborative Project on Enhanced Oil Recovery Agreement
Main Research Area: Technical/natural sciences
Conference: Annual workshop of the IEA Collaborative Project on Enhanced Oil Recovery Agreement, Regina, Canada, 01/01/2003
Source: orbit
Source-ID: 41391
Publication: Research › Conference abstract in proceedings – Annual report year: 2003

Chemical Product Design - A new multidisciplinary teaching and research activity at Institut for Kemiteknik
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.
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.

**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.

**General information**

State: Published
Organisations: Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering, Center for Energy Resources Engineering
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, methylecyclohexane (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, 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
  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
Viscosity Study of Hydrocarbon Fluids at Reservoir Conditions Modeling and Measurements

Thermodynamics of the multicomponent vapor-liquid equilibrium under capillary pressure difference

We discuss the two-phase multicomponent equilibrium, provided that the phase pressures are different due to the action of capillary forces. We prove the two general properties of such an equilibrium, which have previously been known for a single-component case, however, to the best of our knowledge, not for the multicomponent mixtures. The importance is emphasized on the space of the intensive variables P, T and μ(i), where the laws of capillary equilibrium have a simple geometrical interpretation. We formulate thermodynamic problems specific to such an equilibrium, and outline changes to be introduced to common algorithms of flash calculations in order to solve these problems. Sample calculations show large variation of the capillary properties of the mixture in the very neighborhood of the phase envelope and the restrictive role of the spinodal surface as a boundary for possible equilibrium states with different pressures. (C) 2001 Elsevier Science B.V. All rights reserved.
On the nonequilibrium segregation state of a two-phase mixture in a porous column
The problem of segregation of a two-phase multicomponent mixture under the action of thermal gradient, gravity and capillary forces is studied with respect to component distribution in a thick oil-gas-condensate reservoir. Governing equations are derived on the basis of nonequilibrium thermodynamics. A steady state of the two-phase mixture with nonzero diffusion fluxes and exchange between phases is described. In the case of binary mixtures analytical formulae for saturation, component distribution and flow in the two-phase zone are obtained.
Projects:

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)
Project

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
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 Ressources 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

Wood Coatings
Center for Energy Resources Engineering
Department of Chemical and Biochemical Engineering
CERE – Center for Energy Ressources 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)

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: 50893
Project Manager, academic:
Fosbøl, Philip Loldrup (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 Manager, academic:
Fosbøl, Philip Loldrup (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.
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).

Reson
Funded by Højteknologifonden

Ph.D. Advanced Course on Thermodynamic Models: Fundamentals & Computational Aspects
Funded by: Deltagerbetaling
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

CLEO Forskningsprojekt
Funded by TNO
DOC 08/03100

Under lukning

CHIGP DONG
Funded by DONG Energy
DOC 10/00681
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 Ressources Engineering
Period: 01/09/2009 → 31/08/2012
Number of participants: 1
Acronym: ParPor
Project ID: 50711
Project Manager, academic:
Shapiro, Alexander (Intern)

PhD Summer School
Center for Energy Resources Engineering
Department of Chemical and Biochemical Engineering

CERE – Center for Energy Ressources Engineering
Period: 01/01/2009 → 31/12/2015
Number of participants: 1
Project ID: 50671
Project Manager, academic:
Shapiro, Alexander (Intern)

Smart Waterflooding in Carbonate Reservoirs
Center for Energy Resources Engineering
Department of Chemical and Biochemical Engineering

CERE – Center for Energy Ressources Engineering
Period: 01/01/2009 → 28/02/2012
Number of participants: 2
Phd Student:
Zahid, Adeel (Intern)
Main Supervisor:
Thomsen, Kaj (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)

CHIGP Statoil
Funded by Statoil
Center for Energy Resources Engineering
Department of Chemical and Biochemical Engineering
CERE – Center for Energy Ressources Engineering
Period: 03/07/2003 → 31/12/2014
Number of participants: 1
Project ID: 50264
Project Manager, academic:
Kontogeorgis, Georgios (Intern)

Activities:

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
18/05/2017 → 21/05/2017
Bucharest, Romania
Activity: Talks and presentations › Conference presentations

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 Ressources Engineering

Description
Oral Presentation by Ardi Hartono, Fahad Saleem, Muhammad Waseem Arshad, Muhammad Usmana and Hallvard F. Svendsen
Documents:
prod2137141562601.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
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 Ressources 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
Rafiqul Gani (Lecturer)
Department of Chemical and Biochemical Engineering
Computer Aided Process Engineering Center
Center for Energy Resources Engineering
CERE – Center for Energy Ressources 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

Post Combustion CCS activities at Center for Energy Resources Engineering: DTU Climate Centre Seminar on CCS
Period: 22 Sep 2011
Philip Loldrup Fosbøl (Speaker)
Department of Chemical and Biochemical 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 → …
Negar Sadegh (Speaker)
Department of Chemical and Biochemical Engineering
CERE – Center for Energy Resources Engineering

Thermodynamic modeling of sour gas cleaning process with alkanolamines: ESAT 01/06/2011 → …
Saint Petersburg, Russian Federation
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: Presented at (oral presentation) CERE discussion meeting, Hillerød
Period: 1 Jan 2011 → …
Negar Sadegh (Speaker)
Department of Chemical and Biochemical Engineering
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
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 → …
Kaj Thomsen (Speaker)
Department of Chemical and Biochemical Engineering
CERE – Center for Energy Resources Engineering
Center for Energy Resources Engineering