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Publications:

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. CT-scanning, X-ray diffraction (XRD), backscatter electron microscopy images (BSEM), mercury injection capillary pressure (MICP) curves and specific surface analysis (BET) reveal the mineralogy and texture of the rock samples before and after the injection. 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.

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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.
Calculation of simultaneous chemical and phase equilibrium by the method of Lagrange multipliers

The purpose of this work is to develop a general, reliable and efficient algorithm, which is able to deal with multiple reactions in multiphase systems. We selected the method of Lagrange multipliers to minimize the Gibbs energy of the system, under material balance constraints. Lagrange multipliers and phase amounts are the independent variables, whose initialization is performed by solving a subset of the working equations. This initialization is the unconstrained minimization of a convex function and it is bound to converge. The whole solution procedure employs a nested loop with Newton iteration in the inner loop and non-ideality updated in the outer loop, thus giving an overall linear convergence rate. Stability analysis is used to introduce additional phases sequentially so as to obtain the final multiphase solution. The procedure was successfully tested on vapor-liquid equilibrium (VLE) and vapor-liquid-liquid equilibrium (VLLE) of reaction systems.

General information
State: Published
Organisations: Department of Chemistry, Department of Chemical and Biochemical Engineering, Technical University of Denmark
Authors: Tsanas, C. (Ekstern), Stenby, E. H. (Intern), Yan, W. (Intern)
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Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Comparison of GERG-2008 and simpler EoS models in calculation of phase equilibrium and physical properties of natural gas related systems

Accurate description of thermodynamic properties of natural gas systems is of great significance in the oil and gas industry. For this application, non-cubic equations of state (EoSs) are advantageous due to their better density and
compressibility description. Among the non-cubic models, GERG-2008 is a new wide-range EoS for natural gases and other mixtures of 21 natural gas components. It is considered as a standard reference equation suitable for natural gas applications where highly accurate thermodynamic properties are required. Soave's modification of Benedict-Webb-Rubin (Soave-BWR) EoS is another model that despite its empirical nature, provides accurate density description even around the critical point. It is much simpler than GERG-2008 and easier to handle and generalize to reservoir oil fluids. This study presents a comprehensive comparison between GERG-2008 and other cubic (SRK and PR) and noncubic EoSs (Soave-BWR and PC-SAFT) with a focus on Soave-BWR in description of pure components density and compressibility in a wide temperature and pressure range, calculation of binary Vapor-Liquid-Equilibria (VLE) and density, prediction of multicomponent phase envelopes and gas compressibility factor. In addition, the performance of GERG-2008 is compared with that of cubic and non-cubic models in calculation of thermal properties such as heat capacity and Joule-Thomson coefficient for pure components and multicomponent mixtures over a wide pressure and temperature range. The results are compared with available experimental data in the literature and special emphasis has been given to the reverse Joule-Thomson effects at high pressure high temperature (HPHT) conditions. © 2016 Elsevier B.V. All rights reserved.
Density and Compressibility of Multicomponent n-Alkane Mixtures up to 463 K and 140 MPa

Density measurements of two ternary alkane 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 were performed in the temperature range from (278.15 to 463.15) K and pressures up to 140 MPa. The isothermal compressibility values of these mixtures were obtained by differentiation from a Tait-type fitting of experimental densities as a function of temperature and pressure. Excess volume of the studied mixtures was also determined. Four different equations of state, that is, Soave–Redlich–Kwong (SRK), Peng–Robinson (PR), Perturbed Chain Statistical Associating Fluid Theory (PC-SAFT), and Soave-Benedict-Webb-Rubin (Soave-BWR) were used for predicting the experimental density values as well as the excess volumes.

General information
State: Accepted/In press
Organisations: Department of Chemistry, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering, Technical University of Denmark
Authors: Regueira, T. (Intern), Glykioti, M. (Ekstern), Stenby, E. H. (Intern), Yan, W. (Intern)
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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
A new experimental set-up and methodology for the measurement of ZnS solubility in aqueous solutions at 40, 60 and 80 °C (atmospheric pressure) is presented. The methodology implemented includes the preparation of the samples in a reduced oxygen atmosphere, particle size analysis of ZnS, quality control of the analytical technique and evaluation of equilibration time. ZnS solubility analyses were run for prolonged times (up to 11 days) to ensure that equilibrium conditions were met. The equilibration time was explored at three temperatures (40, 60 and 80 °C) observing small variations in the time required to reach the solid–liquid equilibrium at each temperature. Equilibrium was reached within 72
h. The concentration of zinc and of total sulfur were determined using Inductively Coupled Plasma Optical Emission Spectroscopy (ICP-OES). The experimental solubility data show an exponential dependency of the solubility with respect to temperature. An increase of 40 °C results in an increase of roughly 12 times for the solubility of ZnS.

**General information**

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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:* Carolina Figueroa Murcia, D. (Intern), Fosbøl, P. L. (Intern), Thomsen, K. (Intern), Stenby, E. H. (Intern)

*Pages:* 1805-1817

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*Main Research Area:* Technical/natural sciences

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*Scopus rating (2016):* CiteScore 1.31 SJR 0.441 SNIP 0.606

*Web of Science (2016):* Indexed yes

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*Scopus rating (2015):* SJR 0.426 SNIP 0.717 CiteScore 1.26

*Web of Science (2015):* Indexed yes

*BFI (2014):* BFI-level 1

*Scopus rating (2014):* SJR 0.493 SNIP 0.896 CiteScore 1.28

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*Scopus rating (2013):* SJR 0.485 SNIP 0.805 CiteScore 1.25

*ISI indexed (2013):* ISI indexed yes

*BFI (2012):* BFI-level 1

*Scopus rating (2012):* SJR 0.505 SNIP 0.815 CiteScore 1.25

*ISI indexed (2012):* ISI indexed yes

*BFI (2011):* BFI-level 1

*Scopus rating (2011):* SJR 0.439 SNIP 0.838 CiteScore 1.31

*ISI indexed (2011):* ISI indexed yes

*BFI (2010):* BFI-level 1

*Scopus rating (2010):* SJR 0.559 SNIP 0.809

*BFI (2009):* BFI-level 1

*Scopus rating (2009):* SJR 0.914 SNIP 1.05

*Web of Science (2009):* Indexed yes

*BFI (2008):* BFI-level 1

*Scopus rating (2008):* SJR 0.833 SNIP 0.84

*Scopus rating (2007):* SJR 0.715 SNIP 0.893

*Scopus rating (2006):* SJR 0.62 SNIP 0.857

*Scopus rating (2005):* SJR 0.53 SNIP 0.919

*Scopus rating (2004):* SJR 0.681 SNIP 1.088

*Scopus rating (2003):* SJR 0.565 SNIP 1.023

*Scopus rating (2002):* SJR 0.555 SNIP 0.929

*Scopus rating (2001):* SJR 0.572 SNIP 0.988

*Web of Science (2001):* Indexed yes

*Scopus rating (2000):* SJR 0.578 SNIP 1.139

*Scopus rating (1999):* SJR 0.593 SNIP 0.97
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.
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.

**Extension of modified RAND to multiphase flash specifications based on state functions other than \((T,P)\)**

**General information**
- **State:** Published
- **Organisations:** Department of Chemistry, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources 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
Flooding of North Sea chalk and greensand cores with specific brines

General information
State: Published
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Publication date: 2017
Event: Poster session presented at 19th European Symposium on Improved Oil Recovery, Stavanger, Norway.
Main Research Area: Technical/natural sciences
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Source: PublicationPreSubmission
Source-ID: 140684892
Publication: Research - peer-review › Poster – Annual report year: 2017

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

General information
State: Published
Organisations: Department of Chemistry, Center for Energy Resources Engineering, CERE – Center for Energy Resources Engineering
Authors: Varzandeh, F. (Intern), Stenby, E. H. (Intern), Yan, W. (Intern)
Number of pages: 15
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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
Heat capacity and Joule-Thomson coefficient of selected \( n \)-alkanes at 0.1 and 10 MPa in broad temperature ranges

Isobaric heat capacity of six \( n \)-alkanes, i.e. \( n \)-hexane, \( n \)-octane, \( n \)-decane, \( n \)-dodecane, \( n \)-tetradecane and \( n \)-hexadecane, was determined with a Calvet type differential heat-flux calorimeter at 0.1 and 10 MPa in a broad temperature range. The
measured isobaric heat capacity data were combined with the literature density data for these n-alkanes to determine the corresponding Joule-Thomson coefficients. Four different EoSs, Soave-Redlich-Kwong, Peng-Robinson, Perturbed Chain Statistical Associating Fluid Theory, and Soave-Benedict-Webb-Rubin, were used to model the heat capacities and Joule-Thomson coefficients. Moreover, the Joule-Thomson inversion curves for these n-alkanes were also calculated by the four EoSs.

**General information**

State: Published

Organisations: Department of Chemistry

Authors: Regueira Muñiz, T. (Intern), Varzandeh, F. (Intern), Stenby, E. H. (Intern), Yan, W. (Intern)

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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

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BFI (2014): BFI-level 1

Scopus rating (2014): SJR 1.224 SNIP 1.306 CiteScore 2.59

Web of Science (2014): Indexed yes

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ISI indexed (2013): ISI indexed yes

Web of Science (2013): Indexed yes

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Scopus rating (2012): SJR 1.221 SNIP 1.181 CiteScore 2.41

ISI indexed (2012): ISI indexed yes

Web of Science (2012): Indexed yes

BFI (2011): BFI-level 1

Scopus rating (2011): SJR 1.24 SNIP 1.307 CiteScore 2.44

ISI indexed (2011): ISI indexed yes

Web of Science (2011): Indexed yes

BFI (2010): BFI-level 1

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BFI (2009): BFI-level 1

Scopus rating (2009): SJR 1.116 SNIP 1.355

BFI (2008): BFI-level 1

Scopus rating (2008): SJR 1.414 SNIP 1.269

Scopus rating (2007): SJR 1.264 SNIP 1.176

Scopus rating (2006): SJR 1.116 SNIP 1.415

Web of Science (2006): Indexed yes

Scopus rating (2005): SJR 0.913 SNIP 1.277

Web of Science (2005): Indexed yes

Scopus rating (2004): SJR 0.847 SNIP 1.124

Scopus rating (2003): SJR 0.726 SNIP 0.986
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-dodecane and methane/n-butane/n-decane, 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.

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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
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
Microfabricated Nanofluidic cells for in situ liquid TEM

Over the last decade, transmission electron microscopy (TEM) has been revolutionized not only by the introduction of new and very sophisticated hardware for improved resolution, such as aberration correctors and monochromators, but also by the improvement of new methods that have provided more than structural information of materials. In this regard, in situ liquid cell electron microscopy (EM) is one of the new emerging methods that gained a lot of attention by making possible to observe processes and samples in liquid environments within the chamber of an electron microscope. The main focus of this PhD project is to improve the technologies behind liquid cell TEM by developing a novel and robust liquid cell device able to increase the control over the liquid layer thickness, essential for good imaging conditions. A new type of nanofluidic cell has been created with an architecture based on wafer bonding of Atomic layer deposited (ALD) Al₂O₃ on Si₃N₄ membranes. With the improved liquid layer thickness control, we use the devices to measure the electron mean free path in water which is a fundamental aspect of TEM studies, and present the high-resolution TEM capabilities of the nanofluidic cell. Furthermore, the first findings on nanoparticle (NP) growth in this particular nanochannel system are presented that also opens up for new types of liquid cell studies with laminar flow.
These results demonstrate the capability of the novel nanofluidic cell to provide ultra-thin liquid layers, allowing quantitative and high-precision acquisition of liquid thickness maps, high resolution observations and meaningful information about synthesis of NPs from metal precursor solutions in confined space.

Finally, a new concept device based on a Si$_3$N$_4$ membrane for plunge freezing fixation, which enables ultra-fast cooling rates, is presented.

**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.
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. We found that the non-cubic models are much better than the cubics in density, compressibility, heat capacity and Joule-Thomson coefficient calculation of the well defined light and heavy components in reservoir fluids over a wide temperature and pressure range, GERG-2008 being the best with the lowest deviation among all EoS models. GERG-2008 however gives very large deviations for bubble point pressure calculation of some heavy and asymmetric binary systems such as n-butane + n-nonane system. This suggests that this EoS and its binary interaction parameters could still be improved for some of the binary pairs. Soave-BWR gives the closest prediction of the thermal properties to that of GERG-2008 among other EoSs tested in this study. The binary VLE calculation showed that PC-SAFT and Soave-BWR are similar to SRK and PR in correlating the important binary pairs in reservoir fluids. Although Soave-BWR and PC-SAFT give smaller average kij values than SRK and PR, they are more sensitive to the change in kij. Phase envelope prediction of synthetic gases showed that all the EoS models were similar for not too asymmetric synthetic gases, with or without the optimal kij values for SRK, PR, PC-SAFT and Soave-BWR. For highly asymmetric synthetic mixtures, Soave-BWR and GERG-2008 tend to predict phase envelopes different from other models where as none of the tested models give satisfactory predictions. For heat capacity and Joule-Thomson coefficients, GERG-2008 and Soave-BWR give the closest predictions. All the evaluated EoS models tend to predict a nearly constant Joule-Thomson coefficient at high pressures. For typical reservoir temperatures, the constant is around -0.5 K/MPa. For non-cubic models like PC-SAFT the characterization method is less mature than the cubic models. A reservoir fluid characterization method for PC-SAFT has been proposed by combining Pedersen’s method with a newly developed set of correlations for the PC-SAFT model parameters m, m/k and mσ3. 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 17EoS-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 along 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 evaluate 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.
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.
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 ζ 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 ζ 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 ζ 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.

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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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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 Tamman-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.
General Approach to Characterize Reservoir Fluids Using a Large PVT Database

Global increase in oil demand has resulted in the need for exploring remote and harsh locations where a considerable portion of them are at extreme reservoir temperatures and pressures. Accurate calculation of properties of gas and oil at high pressures and high temperatures (HPHT) is a more prominent issue. Non-cubic Equation of State (EoS) models are an attractive option due to their better description of density and compressibility over a wide temperature and pressure range. Application of these models to reservoir fluids requires development of the corresponding fluid characterization methods. We proposed a general approach to develop correlations for model parameters and applied it to the characterization for the PC-SAFT EoS. The approach consists in first developing the correlations based on the DIPPR database, and then adjusting the correlations based on a large PVT database. The adjustment was made to minimize the deviation in key PVT properties like saturation pressures, densities at reservoir temperature and Stock Tank Oil (STO) densities, while keeping the n-alkane limit of the correlations unchanged. As an improvement of a previously suggested characterization method, the approach gives better PVT calculation results for the tested systems. Comparison was also made between PC-SAFT with the proposed characterization method and other EoS models. The proposed approach can be applied to other EoS models for improving their fluid characterization. Besides, the challenges with PNA based characterization methods are discussed.

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Release of Crude Oil from Silica and Calcium Carbonate Surfaces: On the Alternation of Surface and Molecular Forces by High- and Low-Salinity Aqueous Salt Solutions

Adsorption and desorption of a North Sea crude oil to silica and calcium carbonate surfaces were studied by a quartz crystal microbalance, while the bare surfaces and adsorbed oil layers were characterized by atomic force microscopy and contact angle measurements. Water contact angles were measured on the bare surfaces, surfaces with an adsorbed oil layer, and surfaces after being exposed to aqueous salt solutions. This showed that the silica surface became more hydrophobic after oil adsorption, while the wettability of the calcium carbonate surface was not significantly changed by adsorption of an oil layer. A surface energy component analysis based on the acid base theory showed that oil adsorption on the surfaces depends upon apolar, acidic, and basic oil components of the crude oil and that the adsorbed oil components differ for adsorption to silica and calcium carbonate. Desorption of the crude oil was investigated by exposing the surfaces with an adsorbed oil layer to a series of NaCl and CaCl2 solutions of decreasing salt concentrations. Here, it was found that the oil release from silica was achieved only by injections of low-salinity solutions, and it is suggested that this observation is due to an expansion of the electrical double layer. The oil release from calcium carbonate was achieved...
by injection of both high- and low-salinity solutions of NaCl but not injection of a high-salinity solution of CaCl₂. These observation are attributed to dissolution of calcium carbonate or reduction in ion bridging in the presence of high-salinity NaCl, while the low-salinity effect again was attributed to an expansion of the electrical double layer.
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.
Densities of the Binary Systems n-Hexane + n-Decane and n-Hexane + n-Hexadecane up to 60 MPa and 463 K

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

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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.

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 and 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.
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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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.

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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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.
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.
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 tielines must be identified.

Calculation of these intersecting tielines 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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- BFI (2008): BFI-level 2
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- Web of Science (2008): Indexed yes
- Scopus rating (2007): SJR 1.105 SNIP 1.239
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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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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, H₂SCH₄-MDEA-H₂O systems and the constituent binary subsystems of the mentioned mixtures. The experimental part of the project includes vapor-liquid equilibrium measurements for CO₂-MDEAH₂O and CO₂-MDEA-PZ-
H$_2$O at atmospheric pressure, high pressure vapor-liquid equilibrium experiments for H$_2$S-CH$_4$-MDEA-H$_2$O, 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.
Composition of in situ burn residue as a function of weathering conditions

Troll B crude oil was weathered under Arctic conditions with different ice coverage: open water, 50% ice and 90% ice. Samples (100 mL) were taken during the experiment and tested for ignitability in a burning cell. From each burning a residue sample was taken for analysis. The burning process removed the light compounds eluting before C13. No effect from the prior weathering time or the different ice coverage was seen in the burn residue composition. The content of selected Poly Aromatic Hydrocarbons (PAHs) was determined and it was noted that the concentration of PAHs with more than 4 rings were increased. The source origin of the PAHs was investigated by use of relative ratios of PAH isomers and indicated that some formation of PAHs was additionally taking place during burning. © 2012 Elsevier Ltd.
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 VLLLE 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.
Inverse Problems in Geosciences: Modelling the Rock Properties of an Oil Reservoir

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

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

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

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

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

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

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

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.
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.

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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/m³ and a sensitivity of 16 Hz/kg/m³. 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.
Solving inverse problems through a smooth formulation of multiple-point geostatistics

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

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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.

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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.
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.
Calculation of minimum miscibility pressure using fast slimtube simulation

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

Comparing ignitability for in situ burning of oil spills for an asphaltenic, a waxy and a light crude oil as a function of weathering conditions under arctic conditions

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

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CO₂ Capture from Flue gas using Amino acid salt solutions

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

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

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

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

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

The chapters of this thesis are organized as follows:

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

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

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

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

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

Chapter 6 concerns a CO₂ solubility study using the apparatus based on the semi-flow method; CO₂ solubility were examined in aqueous solutions of MEA and the five amino acid salts, with concentrations between 2 and 8 molal and temperatures around 298 K, 333 K and 323 K.

Chapter 7 describes a 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.

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Enhanced Oil Recovery with Surfactant Flooding

Enhanced oil recovery (EOR) is being increasingly applied in the oil industry and several different technologies have emerged during the last decades in order to optimize oil recovery after conventional recovery methods have been applied. Surfactant flooding is an EOR technique in which the phase behavior inside the reservoir can be manipulated by the injection of surfactants and co-surfactants, creating advantageous conditions in order to mobilize trapped oil. Correctly designed surfactant systems together with the crude oil can create microemulsions at the interface between crude oil and water, thus reducing the interfacial tension (IFT) to ultra low (0.001 mN/m), which consequently will mobilize the residual oil and result in improved oil recovery. This EOR technology is, however, made challenging by a number of factors, such as the adsorption of surfactant and co-surfactant to the rock during the injection and chromatographic separation of the surfactant and co-surfactant in the reservoir. Therefore it would be a significant step forward to develop single surfactant systems, as this would minimize the consequences of adsorption and separation. Furthermore the surfactants must be resistant to and remain active at reservoir conditions such as high temperatures, pressures and salinities. Understanding the underlying mechanisms of systems that exhibit liquid-liquid equilibrium (e.g. oil-brine systems) at reservoir conditions is an area of increasing interest within EOR. This is true both for complex surfactant systems as well as for oil and brine systems. It is widely accepted that an increase in oil recovery can be obtained through flooding, whether it is simple waterflooding, waterflooding where the salinity has been modified by the addition or removal of specific ions (so-called "smart" waterflooding) or surfactant flooding.

High pressure experiments have been carried out in this work on a surfactant system (surfactant/ oil/ brine) and on oil/ seawater systems (oil/ brine). The high pressure experiments were carried out on a DBR JEFRI PVT cell, where a glass window allows observation of the phase behavior of the different systems at various temperatures and pressures inside the high pressure cell. Phase volumes can also be measured visually through the glass window using precision equipment.

The surfactant system for which an experimental study was carried out consisted of the mixture heptane, sodium dodecyl sulfate (SDS)/ 1-butanol/ NaCl/ water. This system has previously been examined at ambient pressures and temperatures but has been extended here to pressures up to 400 bar and to slightly higher temperatures (40 °C, 45 °C and 50 °C). Experiments were performed at constant salinity (6.56 %), constant surfactant-alcohol ratio (SAR) but with varying water-oil ratios (WOR). At all temperatures it was very clear that the effect of pressure was significant. The system changed from the two phase region, Winsor II, to the three phase region, Winsor III, as pressure increased. Increasing pressures also caused a shift from the three phase region (Winsor III), to a different two phase region, (Winsor I). These changes in equilibrium phase behavior were also dependent on the composition of the system. A number of different compositions of the surfactant system were studied. The effect of increased pressure became more significant when combined with increasing temperature. The experiments performed on the oil/ seawater systems were similar to the high pressure experiments for the surfactant system discussed above. Oil was contacted with different brine solutions with varying sulfate concentrations at a WOR of 70/30. A series of experiments were performed on two crude oils; a Latin American crude oil and a Middle East crude oil. The two crude oils showed significantly different phase behavior when exposed to elevated temperatures and pressures. The Latin American crude showed a decrease in oil viscosity with an increase in sulfate concentration in the brine solution after contacting in the PVT cell. The Middle East crude oil formed emulsions in the PVT cell with increasing temperature and pressure which was more pronounced at higher sulfate concentrations. Further characterization of the two crude oils using gas chromatography and SARA analysis confirmed that the heavier components in the crude oils, (in the case of the Latin American crude oil), are correlated to the observed decrease of viscosity, where the viscosity decrease may be explained from change of the shape of the heavy components with the increase in sulfate concentration after contacting at high pressures and temperatures. A third model system consisting of heptane and seawater solutions was also studied. This system formed emulsions in the PVT cell similar to the Middle East crude oil, which indicates that the lighter components in the Middle East crude oil (compared to the Latin American crude oil) are responsible for the observed formation of emulsions.

The final part of the thesis is a phase behavior modeling study of alkane/ alkanol/ water systems relevant for surfactant flooding. Existing thermodynamic models, such as equations of state, while able to predict and correlate phase equilibrium in two liquid phases (with varying degrees of success) cannot account for the formation of a microemulsion phase. The presence of electrolytes in the surfactant systems further complicates the problem, and the incorporation of electrolytes into equations of state is a problem that, while old, has not been satisfactorily solved. Furthermore the effect of pressure is presently not well accounted for. The simplified PC-SAFT equation of state is used to model the phase behavior of several binary systems. Typically, introducing a small binary interaction parameter, kij, results in good correlations. However, the
interaction parameter must be fitted to each individual binary system. A glycol ether/water binary system was also included in the phase equilibrium modeling study. This system is so difficult to model adequately that an additional binary interaction parameter, $lij$, was introduced to see if the correlations of this system could be improved—especially with regard to the significant effect of pressure on the phase behavior. It was concluded that this additional binary parameter was not sufficient to substantially improve the performance of the model.

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

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

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High Order Adjoint Derivatives using ESDIRK Methods for Oil Reservoir Production Optimization

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

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Organisations: Center for Energy Resources Engineering, Department of Informatics and Mathematical Modeling, Scientific Computing, Department of Chemistry
Managing Injected Water Composition To Improve Oil Recovery: A Case Study of North Sea Chalk Reservoirs

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

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Scopus rating (2015): CiteScore 3.34
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BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 3.52
ISI indexed (2013): ISI indexed yes
There is a recent interest to solve multiphase negative flash problems where the phase amounts can be negative for normal positive feed composition. Solving such a negative flash problem using successive substitution needs an inner loop for phase distribution calculation at constant fugacity coefficients. It is shown that this inner loop, named here as multiphase negative flash for ideal solutions, can be solved either by Michelsen's algorithm for multiphase normal flash, or by its variation which uses F−1 phase amounts as independent variables. In either case, the resulting algorithm is actually simpler than the corresponding normal flash algorithm. Unlike normal flash, multiphase negative flash for ideal solutions can diverge if the feasible domain for phase amounts is not closed. This can be judged readily during the iteration process. The algorithm can also be extended to the partial negative flash situation where several phase amounts must be non-negative and at least one phase amount can be negative.

On multiphase negative flash for ideal solutions

There is a recent interest to solve multiphase negative flash problems where the phase amounts can be negative for normal positive feed composition. Solving such a negative flash problem using successive substitution needs an inner loop for phase distribution calculation at constant fugacity coefficients. It is shown that this inner loop, named here as multiphase negative flash for ideal solutions, can be solved either by Michelsen's algorithm for multiphase normal flash, or by its variation which uses F−1 phase amounts as independent variables. In either case, the resulting algorithm is actually simpler than the corresponding normal flash algorithm. Unlike normal flash, multiphase negative flash for ideal solutions can diverge if the feasible domain for phase amounts is not closed. This can be judged readily during the iteration process. The algorithm can also be extended to the partial negative flash situation where several phase amounts must be non-negative and at least one phase amount can be negative.

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BFI (2013): BFI-level 2
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Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 1.193 SNIP 1.301
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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
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 results to experimental observations, uncertainty and sensitivity analysis of the new models, and realizing the pore-scale physics in network models.

This thesis has been compiled in such a way that each chapter arises from a self-contained study targeting a particular problem of colloid filtration: (1) Recent advances in colloids filtration theory; (2) Non-Fickian Transport and heterogeneous attachment of colloids; (3) Uncertainty and sensitivity analysis of models for non-Fickian transport and heterogeneous attachment; (4) Prediction of injectivity decline during waterflooding; (5) Colloid migration and recapture; (6) Induced colloid migration for enhanced oil recovery; (7) Estimating filtration coefficients for straining.

These studies have been separately published as journal papers, conference papers and book chapters. Nevertheless, they are not independent of one another but logically connected. The connections and main findings can be summarized as follows:

1. The discrepancies between the classical colloid filtration theory and experimental observations have been overviewed in Chapter 1. Many of them are observed under unfavorable attachment conditions, such as hyperexponential and non-monotonic deposition profiles. Such behavior of colloids is attributed to the heterogeneous attachment (Chapters 2 and 3) and the migration of colloids (Chapter 5), respectively.

2. A second reason for the deposition hyperexponentiality is the non-Fickian transport due to the heterogeneity of porous media. It also explains the dispersed and asymmetrical breakthrough curves of tracers in natural porous media (Chapters 2 and 3). Chapter 2 shows that the elliptic equation can be applied to capture the non-Fickian behaviors of colloids and tracers in porous media. It is closely followed by Chapter 3, the uncertainty and sensitivity analysis of the model predictions and the parameter estimation. Suggestions for experimental design for accurate determination of the model parameters are also provided.

3. Chapters 2 and 3 form a thorough study of the integral model for colloid filtration with non-Fickian transport and heterogeneous attachment. They are followed by the study of applying of such a model in the petroleum industry to predict injectivity decline during waterflooding in Chapter 4. However, the non-Fickian behavior of particles around the injection well is shown not to be significant. The reasons are that the temporal dispersion term is inverse proportional to the particle velocity and that the particle velocity is higher close to the well than that far away from the well.

4. The criterion of an attached colloid particle to be re-entrained by the hydrodynamic drag into the bulk fluid is the torques of detachment exceeding those of attachment. Bearing such a criterion in mind, the erosion of external cake, the migration of surface-associated colloids during one phase flow, and the migration of reservoir fines during two-phase flow are studied in similar fashions (Chapters 4, 5, 6). The erosion of external cakes in the injection wells gives rise to the steady stage of the injectivity and filling rat holes in the well (Chapter 4). The migration of surface-associated colloids gives rise to non-monotonic deposition profiles (Chapter 5). Migration and straining of reservoir fines may enhance oil recovery by increasing the sweep efficiency (Chapter 6).

5. Another important mechanism for particle capture is straining or size exclusion of colloids. Such phenomena are closely tied to the migration of colloids under unfavorable attachment conditions: surface-associated colloids rolling to straining sites (grain-grain contacts, pore throats) in Chapter 5, and the straining of released reservoir fines at pore throats in Chapter 6. However, the straining mechanism is described by nothing more than a straining rate coefficient in these studies. Finally in Chapter 7, a much better understanding of straining is achieved by the study of pore scale physics in a network model. The filtration coefficient for straining is estimated from the particle size and the pore size distributions. A new capture scheme of straining (minimum capture) is proposed to explain the large penetration depths of colloids in porous media and the power law dependencies of filtration coefficients in the experiments.

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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 CO₂–NH₃–H₂O 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.

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Production Optimization for Two-Phase Flow in an Oil Reservoir

Petroleum reservoirs are subsurface formations of porous rocks with hydrocarbons trapped in the pores. Initially, the reservoir pressure may be sufficiently large to push the fluids to the production facilities. However, as the fluids are produced the pressure declines and production reduces over time. When the natural pressure becomes insufficient, the pressure must be maintained artificially by injection of water. Conventional technologies for recovery leaves more than 50% of the oil in the reservoir. Wells with adjustable downhole flow control devices coupled with modern control technology offer the potential to increase the oil recovery significantly. In optimal control of smart wells, downhole sensor equipment and remotely controlled valves are used in combination with large-scale subsurface flow models and gradient based optimization methods in a Nonlinear Model Predictive Control framework to increase the production and economic value of an oil reservoir. Wether the objective is to maximize recovery or some financial measure like Net Present Value, the increased production is achieved by manipulation of the well rates and bottom-hole pressures of the injection and production wells. The optimal water injection rates and production well bottom-hole pressures are computed by solution of a large-scale constrained optimal control problem. Optimal control settings of injection and production wells are computed by solution of a large scale constrained optimal control problem. We describe a gradient based method to compute the optimal control strategy of the water flooding process. An explicit singly diagonally implicit Runge-Kutta (ESDIRK) method with adaptive stepsize control is used for computationally efficient solution of the model. The gradients are computed by the adjoint method. The adjoint equations associated with the ESDIRK method are solved by integrating backwards in time. The necessary information for the adjoint computation is calculated and stored during the forward solution of the model. The backward adjoint computation then only requires the assembly of this information to compute the gradients.

Smart Waterflooding in Carbonate Reservoirs

During the last decade, smart waterflooding has been developed into an emerging EOR technology both for carbonate and sandstone reservoirs that does not require toxic or expensive chemicals. Although it is widely accepted that different salinity brines may increase the oil recovery for carbonate reservoirs, understanding of the mechanism of this increase is still developing. To understand this smart waterflooding process, an extensive research has been carried out covering a broad range of disciplines within surface chemistry, thermodynamics of crude oil and brine, as well as their behavior in porous media.

The main conclusion of most previous studies was that it is the rock wettability alteration towards more water wetting condition that helps improving the oil recovery. In the first step of this project, we focused on verifying this conclusion. Coreflooding experiments were carried out using Stevens
which has been thoroughly described at atmospheric pressure, is examined at elevated pressure. The effect of obtaining very low interfacial tension, which consequently helps mobilize the trapped oil. In this work a surfactant system, co-surfactants) into the reservoir, in order to create microemulsions at the interface between crude oil and water, thus in this context, surfactant flooding has recently gained interest again. Surfactant flooding is the injection of surfactants (and brines from carbonate core plugs at 90 °C.

Comparison of the incremental oil recovery from Stevens Klint outcrop chalk core plugs with brines without sulfate, as well as brines containing sulfate in different concentrations. The effects of temperature, injection rate, crude oil composition and different sulfate concentrations on the total oil recovery and the recovery rate were investigated. Experimental results clearly indicate improvement of the oil recovery without wettability alteration.

At the second step of this project, we studied crude oil/brine interactions under different temperatures, pressures and salinity conditions in order to understand mechanisms behind the high salinity waterflooding. Our results show, in particular that sulfate ions may help decreasing the crude oil viscosity or formation of, seemingly, an emulsion phase between sulfate-enriched brine and oil at high temperature and pressure. Experimental results indicate that crude oils interact differently with the same brine solutions regarding phase behavior and viscosity measurements. This difference is attributed to the difference in composition of the different crude oils. More experiments are carried out in order to understand mechanisms of the crude oil viscosity reduction and emulsion formation. We observed that a heavy oil (that with a large fraction of heavy components) exhibited viscosity reduction in contact with brine, while a light crude oil exhibited emulsion formation.

Most of reported high salinity waterflooding studies were carried out with outcrop chalk core plugs, and by performing spontaneous imbibition rather than forced flooding. The objective of the third step of this project was to investigate the potential of high salinity waterflooding process by carrying out experiments with reservoir chalk samples. We carried out waterflooding instead of spontaneous imbibition using core plugs with and without aging. The total oil recovery, recovery rate and interaction mechanisms of ions with rock were studied for different injected fluids under different temperatures and wettability conditions. Experimental results demonstrate that the oil recovery mechanism under high salinity seawater flooding at high temperatures is different for the different chalk rocks (outcrop and reservoir), although they have similar surface area and reactivity of the potential determining ions.

In the last decade, laboratory waterflooding experiments and field tests have proven increase in oil recovery from sandstone reservoirs by injecting brine of low salinity. However, this effect has not been thoroughly investigated for carbonates. At the final stage of this project, we have experimentally investigated the oil recovery potential of low salinity water flooding in the carbonate rocks. We used both reservoir carbonate and outcrop chalk core plugs. The flooding experiments were carried out initially with the seawater. Afterwards the contribution to oil recovery was evaluated by sequential injection of various diluted versions of the seawater.

The significance of this work may be summarized in five main findings:
- * Injection of sulfate rich brine may lead to additional recovery from Stevens Klint chalk even under completely water wet conditions. Therefore, increment in oil recovery with sulfate ions cannot be explained just by the rock wettability alteration.
- * Experimental results show that sulfate ions may help decreasing the crude oil viscosity when brine is contacted with oil under high temperature and pressure. We have also observed formation of an emulsion-like phase between oil and brine with increased sulfate ion concentration under high temperature and pressure. The viscosity decrease and formation of an emulsion 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.
- * Crude oil/brine interaction study suggests that viscosity reduction for crude oil in contact with brine is connected to the presence of heavy components in the crude oil, while formation of emulsions with brine is a phenomenon related to the presence of lighter components in the crude oil.
- * The reservoir chalk rocks showed relatively less effect of temperature and sulfate ions concentration on oil recovery as compared to Stevens Klint outcrop chalk. This indicates that the rock may also determine whether the effect of temperature and high salinity brine on the recovery is observed.
- * Migration of fines and dissolution of rock particles are possible mechanisms of oil recovery increment with low salinity brines from carbonate core plugs at 90 °C.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering
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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.

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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: Sandersen, S. B. (Intern), Stenby, E. H. (Intern), von Solms, N. (Intern)
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BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.803 SNIP 1.116 CiteScore 2.83
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.843 SNIP 1.252 CiteScore 2.81
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Scopus rating (2013): SJR 0.811 SNIP 1.255 CiteScore 2.6
ISI indexed (2013): ISI indexed yes
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Scopus rating (2012): SJR 0.841 SNIP 1.189 CiteScore 2.34
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Scopus rating (2008): SJR 0.886 SNIP 1.041
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Scopus rating (2006): SJR 0.822 SNIP 1.091
Scopus rating (2005): SJR 0.813 SNIP 1.004
Scopus rating (2004): SJR 0.844 SNIP 1.106
Scopus rating (2003): SJR 0.824 SNIP 1.033
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 0.763 SNIP 0.945
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.
Over the last decade, a number of studies have shown SO$_4^{2-}$, Ca$^{2+}$ and Mg$^{2+}$ to be potential determining ions, which may be added to the injected brine for improving oil recovery during waterflooding in chalk reservoirs. However, the understanding of the mechanism leading to an increase in oil recovery is still not clear. In this work, the crude oil/seawater ions interaction at different temperatures, pressures and sulfate ion concentrations is investigated. Our results show that sulfate ions may help decrease the crude oil viscosity when brine is contacted with oil under high temperature and pressure. We have also observed formation of a microemulsion phase between brine and oil with the increase in sulfate ion concentration at high temperature and pressure. In addition, sulfate ions can reduce interfacial tension (IFT) between oil and water. We propose that the decrease in viscosity and formation of a microemulsion phase could be the possible reasons for the observed increase in oil recovery with sulfate ions at high temperature in chalk reservoirs besides the mechanism of the rock wettability alteration, which has been reported in most previous studies.
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.

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
Authors: Lerche, B. M. (Intern), Thomsen, K. (Intern), Stenby, E. H. (Intern)
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CO2 capture using aqueous ammonia: kinetic study and process simulation

Carbon dioxide capture using aqueous ammonia is a post-combustion technology that has shown a good potential. Therefore this process is studied by measuring the rate of absorption of carbon dioxide by aqueous ammonia and by
performing process simulation. The rate of absorption of carbon dioxide by aqueous ammonia solvent has been studied by applying a wetted wall column apparatus. The rate of absorption is crucial regarding the sizing of the absorber columns. The overall mass transfer coefficient has been measured at temperatures from 279 to 304 K for 1 to 10 wt% ammonia solutions at loadings up to 0.6. The results were compared with those found for 30 wt% mono-ethanolamine (MEA) solutions. The capture process was simulated successfully using the simulator Aspen Plus coupled with the extended UNIQUAC thermodynamic model available for the NH3–CO2–H2O system. For this purpose, a user model interface was developed. The heat and electricity requirements were analyzed for a base case configuration, and a preliminary sensitivity analysis was performed on the heat and the electricity requirements and on the ammonia slip from the absorber.

General information
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)
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Scopus rating (2016): CiteScore 1.16 SJR 0.467 SNIP 0.586
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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
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Web of Science (2012): Indexed yes
Scopus rating (2011): SJR 0.918 SNIP 1.505 CiteScore 2.42
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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 Tie-line Distance Based Approximation (TDBA) method to get approximate flash results in the two-phase region. The method uses the distance to a previous tie-line 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.

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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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Distribution of Complex Chemicals in Oil-Water Systems
The deepwater energy sector represents one of the major growth areas of the oil and gas industry today. In order to meet the challenges of hydrate formation, corrosion, scaling and foaming the oil and gas industry uses many chemicals and their use has increased significantly over the years. In order to inhibit gas hydrate formation in subsea pipelines monoethylene glycol (MEG) and methanol are injected in large amounts. It is important to know the distribution of these chemicals in oil and water systems for economical operation of a production facility and to evaluate their impact on marine life. Furthermore distribution of chemicals is important information for downstream processing of oil and gas. The purpose of this project is the experimental measurement and the thermodynamic modeling of distribution of these complex chemicals in oil-water systems.

Traditionally distribution of chemicals in oil-water 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.

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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**

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

**General information**

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

General information
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Organisations: CERE – Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, Friedrich-Alexander University Erlangen-Nuremberg
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BFI (2014): BFI-level 1
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Scopus rating (2011): SJR 0.238 SNIP 0.497 CiteScore 0.42
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BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.21 SNIP 0.344
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.255 SNIP 0.45
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.196 SNIP 0.277
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 0.187 SNIP 0.297
Scopus rating (2006): SJR 0.171 SNIP 0.249
Scopus rating (2005): SJR 0.184 SNIP 0.323
Web of Science (2005): Indexed yes
Experimental measurement and modeling of the rate of absorption of carbon dioxide by aqueous ammonia

In this work, the rate of absorption of carbon dioxide by aqueous ammonia solvent has been studied by applying a newly built wetted wall column. The absorption rate in aqueous ammonia was measured at temperatures from 279 to 304K for 1 to 10wt% aqueous ammonia with loadings varying from 0 to 0.8molCO2/molNH3. The absorption rate in 30wt% aqueous mono-ethanolamine (MEA) was measured at 294 and 314K with loadings varying from 0 to 0.4 as comparison. It was found that at 304K, the rate of absorption of carbon dioxide by 10wt% NH3 solvent was comparable to the rates for 30wt% MEA at 294 and 314K (a typical absorption temperature for this process). The absorption rate using ammonia was however significantly lower at temperatures of 294K and lower as applied in the Chilled Ammonia Process. However, at these low temperatures, the rate of absorption in ammonia has only a small temperature dependency. The rate of absorption decreases strongly with decreasing ammonia concentrations and increasing CO2 loadings. The rate of absorption of carbon dioxide by aqueous ammonia solvent was modeled using the measurements of the unloaded solutions and the zwitter-ion mechanism. The model could successfully predict the experimental measurements of the absorption rate of CO2 in loaded ammonia solutions.

General information
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Organisations: CERE – Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, Department of 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)
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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
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Scopus rating (2013): SJR 2.331 SNIP 3.018 CiteScore 5.66
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
Measurement and modeling of CO2 solubility in NaCl brine and CO2–saturated NaCl brine density

Phase equilibrium for CO2–NaCl brine is of general interest to many scientific disciplines and technical areas. The system is particularly important to CO2 sequestration in deep saline aquifers and CO2 enhanced oil recovery, two techniques discussed intensively in recent years due to the concerns over climate change and energy security. This work is an experimental and modeling study of two fundamental properties in high pressure CO2–NaCl brine equilibrium, i.e., CO2 solubility in NaCl brine and CO2–saturated NaCl brine density. A literature review of the available data was presented first to illustrate the necessity of experimental measurements of the two properties at high pressures. An experimental method for measuring high pressure CO2 solubility in NaCl brine was then developed. With the method, CO2 solubilities in 0, 1, and 5 m NaCl brines were measured at 323, 373, and 413 K from 5 to 40 MPa. The corresponding density data at the same conditions were also measured. For solubility, two models used in the Eclipse simulator were tested: the correlations of Chang et al. and the Søreide and Whitson equation of state (EoS) model. The latter model was modified to improve its performance for high salinity brine. In the density modeling, the correlations of Chang et al., Garcia's correlation, and five different EoS models were tested. Among these models, Garcia's correlation and the ePC-SAFT EoS generally give satisfactory agreement with the experimental measurements. An analysis was also made to show that dissolution of CO2 increases the brine density only if the apparent mass density of CO2 in brine is higher than the brine density at the same conditions.

General information
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Organisations: Center for Energy Resources Engineering, CERE – Center for Energy Ressources Engineering, Department of Chemical and Biochemical Engineering, Technical University of Denmark
Authors: Yan, W. (Intern), Huang, S. (Ekstern), Stenby, E. H. (Intern)
Pages: 1460-1477
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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
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 Resources Engineering, Department of Chemical and Biochemical Engineering, Department of Chemistry, Center for Energy Resources Engineering, Statoil ASA
Authors: Riaz, M. (Intern), Kontogeorgis, G. (Intern), Stenby, E. H. (Intern), Yan, W. (Intern), Haugum, T. (Ekstern), Christensen, K. O. (Ekstern), Løkken, T. V. (Ekstern), Solbraa, E. (Ekstern)

Measurement, CO2 solubility, Modeling, Brine density, NaCl brine

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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 Ressources 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
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Web of Science (2017): Indexed yes
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Scopus rating (2016): CiteScore 2.33 SJR 0.869 SNIP 1.155
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.874 SNIP 0.998 CiteScore 1.99
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 0.982 SNIP 1.248 CiteScore 2.28
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
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.
In this paper, we use nonlinear model predictive control (NMPC) to maximize secondary oil recovery from an oil reservoir by controlling two-phase subsurface porous flow using adjustable down-hole control valves. The resulting optimal control problem is nonlinear and large-scale. We solve this problem numerically using a single shooting sequential quadratic programming (SQP) based optimization method. Explicit singly diagonally implicit Runge-Kutta (ESDIRK) methods are used for integration of the stiff system of differential equations describing the two-phase flow, and the adjoint method is used for sensitivity computations. We report computational experiences and oil recovery improvements for a standard test case.

**General information**

State: Published
Organisations: Scientific Computing, Department of Informatics and Mathematical Modeling, Department of Chemistry, Center for Energy Resources Engineering
Authors: Völcker, C. (Intern), Jørgensen, J. B. (Intern), Thomsen, P. G. (Intern), Stenby, E. H. (Intern)
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Source: orbit
Source-ID: 275828
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**Oil Reservoir Production Optimization using Optimal Control**

Practical oil reservoir management involves solution of large-scale constrained optimal control problems. In this paper we present a numerical method for solution of large-scale constrained optimal control problems. The method is a single-shooting method that computes the gradients using the adjoint method. We use an Explicit Singly Diagonally Implicit Runge-Kutta (ESDIRK) method for the integration and a quasi-Newton Sequential Quadratic Programming (SQP) algorithm for the constrained optimization. We use this algorithm in a numerical case study to optimize the production of oil from an oil reservoir using water flooding and smart well technology. Compared to the uncontrolled case, the optimal operation increases the Net Present Value of the oil field by 10%.
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.
Physical mechanisms of deep bed filtration with application to the problems of petroleum industry

General information
State: Published
Organisations: Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Ressources Engineering, Department of Chemistry
Authors: Yuan, H. (Intern), Shapiro, A. (Intern), Stenby, E. H. (Intern)
Publication date: 2011

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Original language: English
Main Research Area: Technical/natural sciences
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Publication: Research › Sound/Visual production (digital) – Annual report year: 2011

Pressure Effect on Phase Behavior of Surfactant System

General information
State: Published
Organisations: CERE – Center for Energy Ressources Engineering, Department of Chemical and Biochemical Engineering, Department of Chemistry
Authors: Sandersen, S. B. (Intern), von Solms, N. (Intern), Stenby, E. H. (Intern)
Publication date: 2011
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Electronic versions:
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Publication: Research › Poster – Annual report year: 2011

Pressure Effect on Phase Behavior of Surfactant System

General information
State: Published
Organisations: CERE – Center for Energy Ressources Engineering, Department of Chemical and Biochemical Engineering, Department of Chemistry
Authors: Sandersen, 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

Screening of amino acid salts solutions for application in CO2 capture from flue gas.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering, Department of Chemistry, CERE – Center for Energy Ressources Engineering
Authors: Lerche, B. M. (Intern), Stenby, E. H. (Intern), Thomsen, K. (Intern)
Number of pages: 2
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.
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
Publication date: Dec 2010

Publications

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 100bars. 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 2GJ/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
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Main Research Area: Technical/natural sciences

Publications
1D Simulations for Microbial Enhanced Oil Recovery with Metabolite Partitioning

We have developed a mathematical model describing the process of microbial enhanced oil recovery (MEOR). The one-dimensional isothermal model comprises displacement of oil by water containing bacteria and substrate for their feeding. The bacterial products are both bacteria and metabolites. In the context of MEOR modeling, a novel approach is partitioning of metabolites between the oil and the water phases. The partitioning is determined by a distribution coefficient. The transfer part of the metabolite to oil phase is equivalent to its "disappearance", so that the total effect from of metabolite in the water phase is reduced. The metabolite produced is surfactant reducing oil–water interfacial tension, which results in oil mobilization. The reduction of interfacial tension is implemented through relative permeability curve modifications primarily by lowering residual oil saturation. The characteristics for the water phase saturation profiles and the oil recovery curves are elucidated. However, the effect from the surfactant is not necessarily restricted to influence only interfacial tension, but it can also be an approach for changing, e.g., wettability. The distribution coefficient determines the time lag, until residual oil mobilization is initialized. It has also been found that the final recovery depends on the distance from the inlet before the surfactant effect takes place. The surfactant effect position is sensitive to changes in maximum growth rate, and injection concentrations of bacteria and substrate, thus determining the final recovery. Different methods for incorporating surfactant-induced reduction of interfacial tension into models are investigated. We have suggested one method, where several parameters can be estimated in order to obtain a better fit with experimental data. For all the methods, the incremental recovery is very similar, only coming from small differences in water phase saturation profiles. Overall, a significant incremental oil recovery can be achieved, when the sensitive parameters in the context of MEOR are carefully dealt with.

General information
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Organisations: CERE – Center for Energy Ressources Engineering, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Absorber Model for CO2 Capture by Monoethanolamine

The rate-based steady-state model proposed by Gabrielsen et al. (Gabrielsen, J.; Michelsen, M. L.; Kontogeorgis, G. M.; Stenby, E. H. AIChE J. 2006, 52, 10, 3443-3451) for the design of the CO2-2-amino-2-methylpropanol absorbers is adopted and improved for the design of the CO2-monoethanolamine absorber. The influence of the application of different mass transfer correlations on the model's performance is investigated. Analytical expressions for the calculation of the enhancement factor for the second order as well as the pseudo-first-order reaction regime are integrated in the model, and their impact on the model's prediction is compared. The model has been successfully applied to CO2 absorber packed columns and validated against pilot plant data with good agreement.

General information
State: Published
Organisations: CERE – Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Faramarzi, L. (Intern), Kontogeorgis, G. (Intern), Michelsen, M. L. (Intern), Thomsen, K. (Intern), Stenby, E. H. (Intern)
Pages: 3751-3759
Publication date: 2010
Main Research Area: Technical/natural sciences

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BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.1 SJR 0.945 SNIP 1.139
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.949 SNIP 1.146 CiteScore 2.87
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.012 SNIP 1.292 CiteScore 2.85
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 0.982 SNIP 1.243 CiteScore 2.6
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.066 SNIP 1.338 CiteScore 2.56
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.086 SNIP 1.24 CiteScore 2.58
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.047 SNIP 1.165
Web of Science (2010): Indexed yes
Adaptive Step Size Control in Implicit Runge-Kutta Methods for Reservoir Simulation

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Organisations: Scientific Computing, Department of Informatics and Mathematical Modeling, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
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Pages: 509-514
Publication date: 2010

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Source-ID: 259671
Publication: Research - peer-review › Article in proceedings – Annual report year: 2010

Advanced Waterflooding in Carbonate Reservoirs

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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
Event: Poster session presented at 11th International Symposium on Evaluation of Wettability and Its Effect on Oil Recovery, University of Calgary, Alberta, Canada, .
Compositional Simulation of In-Situ Combustion EOR: A Study of Process Characteristics

In order to facilitate the study of the influence of reservoir process characteristics in In-Situ combustion modeling and advance the work of Kristensen et al. in this domain; a fully compositional In-situ combustion (ISC) model of Virtual Kinetic Cell (VKC; single-cell model) for laboratory scale combustion simulation is used. Preceding research work primarily focused on a kinetic model that was based on six components and incorporated four chemical reactions. However, modeling of a thermal process as complex as In-situ combustion requires in-depth understanding of detailed reaction kinetics and multidisciplinary process data. This paper extends the understanding of previous research done in this domain by performing the process simulations to study further the impact of oxidation reactions and combustion reactions of crude oils along with their saturate, aromatic, resin, and asphaltene (SARA) fractions. This incorporates fourteen pseudo components and fourteen reactions (distributed amongst thermal cracking, low temperature oxidation and high temperature oxidation). The paper presents a set of derivative plots indicating that reservoir process characterization in terms of thermal behavior of oil can be well construed in terms of thermo-oxidative sensitivity of SARA fractions. It can be interpreted from the results that operating parameters like air injection rate, oxygen feed concentration and activation energy have significant influence on oil recovery; an increase in air injection rate can lead to cooling of the combustion front and thus decrease oil recovery, while increase in oxygen feed assists combustion and contributes towards improved oil recovery. The critical properties of the pseudo components are not determined experimentally, thus extending significance to fluid characterization. The composition plays a key role e.g. due to asphaltenes being most resistant toward oxidation and saturates being the easiest oxidizable ones.

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Organisations: Department of Chemical and Biochemical Engineering
Authors: Jain, P. (Intern), Stenby, E. H. (Intern), von Solms, N. (Intern)
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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
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ISI indexed (2011): ISI indexed yes
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Explicit Singly Diagonally Implicit Runge-Kutta Methods and Adaptive Stepsize Control for Reservoir Simulation

The implicit Euler method, normally referred to as the fully implicit (FIM) method, and the implicit pressure explicit saturation (IMPES) method are the traditional choices for temporal discretization in reservoir simulation. The FIM method offers unconditionally stability in the sense of discrete approximations, while the IMPES scheme benefits from the explicit treatment of the saturation. However, in terms of controlling the integration error, the low order of the FIM method leads to small integration steps, while the explicit treatment of the saturation may restrict the stepsizes for the IMPES scheme. Current reservoir simulators apply timestepping algorithms that are based on safeguarded heuristics, and can neither guarantee convergence in the underlying equation solver, nor provide estimates of the relations between convergence, integration error and stepsizes. We establish predictive stepsize control applied to high order methods for temporal discretization in reservoir simulation. The family of Runge-Kutta methods is presented and in particular the explicit singly diagonally implicit Runge-Kutta (ESDIRK) method with an embedded error estimate is described. A predictive stepsize adjustment rule based on error estimates and convergence control of the integrated iterative solver is presented. We try to improve the predictive stepsize control through an extended communication between the convergence rate, the error control and the stepsizes. Keywords: Reservoir simulation, implicit Runge-Kutta methods, ESDIRK, Newton-Raphson, convergence control, error control, stepsize selection.

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Organisations: Scientific Computing, Department of Informatics and Mathematical Modeling, Department of Chemistry, Center for Energy Resources Engineering
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Publication date: 2010

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Extensive Comparison of Cubic Plus Association (CPA) and PC-SAFT Equations of State
How to Model CO2 Capture

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Organisations: CERE – Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering
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Pages: 95-96
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Conference: 3. Danski KemiingeniørKonference, Kgs. Lyngby, Denmark, 16/06/2010 - 16/06/2010
Source: orbit
Source-ID: 274744
Publication: Research › Article in proceedings – Annual report year: 2010

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Organisations: Section for Arctic Technology, Department of Civil Engineering, Department of Chemistry, Arctic Technology Centre, SINTEF, Materialer og kjemi
Authors: Fritt-Rasmussen, J. (Intern), Villumsen, A. (Intern), Brandvik, P. J. (Ekstern), Stenby, E. H. (Intern)
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Improved Oil Recovery in Chalk: Wettability Alteration or Something Else?

**General information**
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Improved Oil Recovery in Chalk: Wettability Alteration or Something Else?
In-Situ Phase Identification and Saturation Determination in Carbon Dioxide Flooding of Water Flooded Chalk Using X-Ray Computed Tomography

General information
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Organisations: Department of Chemical and Biochemical Engineering
Authors: Niu, B. (Intern), Yan, W. (Intern), Shapiro, A. (Intern), Stenby, E. H. (Intern)
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Web of Science (2017): Indexed Yes
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Scopus rating (2016): SJR 0.95 SNIP 2.003 CiteScore 3.01
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
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BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.185 SNIP 2.152 CiteScore 2.43
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Scopus rating (2013): SJR 0.993 SNIP 1.773 CiteScore 2.25
ISI indexed (2013): ISI indexed yes
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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
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In-Situ Phase Identification and Saturation Determination in Carbon Dioxide Flooding of Water Flooding Chalk Using X-Ray Computed Tomography

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Authors: Niu, B. (Intern), Yan, W. (Intern), Shapiro, A. (Intern), Stenby, E. H. (Intern)
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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.

### General information

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Organisations: CERE – Center for Energy Ressources Engineering, Department of Chemical and Biochemical Engineering  
Authors: Nielsen, S. M. (Intern), Jessen, K. (Ekstern), Shapiro, A. (Intern), Michelsen, M. L. (Intern), Stenby, E. H. (Intern)  
Number of pages: 11  
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### Microbial Enhanced Oil Recovery - Advanced Reservoir Simulation

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 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.

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Organisations: CERE – Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, Department of Chemistry
Authors: Nielsen, S. M. (Intern), Shapiro, A. (Intern), Stenby, E. H. (Intern), Michelsen, M. L. (Intern)
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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.
Mutual Solubility of MEG, Water and Reservoir Fluid: Experimental Measurements and Modeling using the CPA Equation of State

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Mutual Solubility of MEG, Water and Reservoir Fluid: Experimental Measurements and Modeling using the CPA Equation of State

General information
State: Published
Organisations: CERE – Center for Energy Ressources Engineering, Department of Chemical and Biochemical Engineering
Mutual Solubility of MEG, Water and Reservoir Fluid: Experimental Measurements and Modeling using the CPA Equation of State

Phase equilibria modeling of methanol-containing systems with the CPA and sPC-SAFT equations of state
Post-Combustion Capture of CO2 from Fossil Fueled Power Plants
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%.
Production Optimization for Two-Phase Flow In an Oil Reservoir

General information
State: Published
Organisations: Center for Energy Resources Engineering, Department of Informatics and Mathematical Modeling, Scientific Computing, Department of Chemistry
Authors: Völcker, C. (Intern), Jørgensen, J. B. (Intern), Thomsen, P. G. (Intern), Stenby, E. H. (Intern)
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Main Research Area: Technical/natural sciences
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PVT Modeling of Reservoir Fluids using PC-SAFT EoS and Soave-BWR EOS

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Organisations: CERE – Center for Energy Ressources Engineering, Department of Chemical and Biochemical Engineering
Rate Based Carbon Dioxide Capture Desorption Modelling

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Organisations: CERE – Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering
Authors: Fosbøl, P. L. (Intern), Thomsen, K. (Intern), Stenby, E. H. (Intern)
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Recent Applications of the CPA Equations of State

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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)
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Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 274773
Publication: Research › Poster – Annual report year: 2010

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.

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State: Published
Organisations: CERE – Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Fosbøl, P. L. (Intern), Thomsen, K. (Intern), Stenby, E. H. (Intern)
Pages: 115-135
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Main Research Area: Technical/natural sciences

Publication information
Journal: Corrosion Engineering, Science and Technology
Volume: 45
Solubility of CO₂ in functionalized ionic liquid

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Center for Energy Resources Engineering
Tertiary Carbon Dioxide Flooding of Low Permeable Chalk with In-Situ Saturation Determination using X-Ray Computed Tomography

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

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 slimtube 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.
Towards Predictive Association Theories

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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

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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
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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
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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), Stenby, E. H. (Intern)
Publication date: 2010
Event: Poster session presented at Center for Energy Resources Engineering Discussion Meeting 2010, LO-skolens konferencecenter, Gl. Hellebækvej 70, DK-3000 Helsingør,
Main Research Area: Technical/natural sciences
Source: orbit
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Publication: Research › Poster – Annual report year: 2010

An Equation-of-State Compositional In-Situ Combustion Model: A Study of Phase Behavior Sensitivity
In order to facilitate the study of reactive-compositional porous media processes we develop a virtual kinetic cell (single-cell model) as well as a virtual combustion tube (one-dimensional model). Both models are fully compositional based on an equation of state. We employ the models to study phase behavior sensitivity for in situ combustion, a thermal oil recovery process. For the one-dimensional model we first study the sensitivity to numerical discretization errors and
provide grid density guidelines for proper resolution of in situ combustion behavior. A critical condition for success of in situ combustion processes is the formation and sustained propagation of a high-temperature combustion front. Using the models developed, we study the impact of phase behavior on ignition/extinction dynamics as a function of the operating conditions. We show that when operating close to ignition/extinction branches, a change of phase behavior model will shift the system from a state of ignition to a state of extinction or vice versa. For both the rigorous equation of state based and a simplified, but commonly used, K-value-based phase behavior description we identify areas of operating conditions which lead to ignition. For a particular oil we show that the simplified approach overestimates the required air injection rate for sustained front propagation by 17% compared to the equation of state-based approach.
A New Approach to Modeling Immiscible Two-phase Flow in Porous Media

In this work we present a systematic literature review regarding the macroscopic approaches to modeling immiscible two-phase flow in porous media, the formulation process of the incorporate PDE based on Film Model (viscous coupling), the calculation of saturation profile around the transition zone based on Rapoport-Leas Equation and Film Model, a systematic literature review of the LBM CFD methods including the particle-based LBM and porous-medium-based LBM for multiphase flow, and the sample calculation of particle-based LBM in a random porous medium. Finally we come to present a new approach to modeling immiscible two-phase flow in porous media. The suggested approach to immiscible two-phase flow in porous media describes the dispersed mesoscopic fluids’ interfaces which are highly influenced by the injected interfacial energy and the local interfacial energy capacity. It reveals a new possibility of modeling two-phase flow through energy balance. The saturation profile generated through the suggested approach is different from those through other approaches.

Application of the CPA equation of state to reservoir fluids in presence of water and polar chemicals

The complex phase equilibrium between reservoir fluids and associating compounds like water, methanol and glycols has become more and more important as the increasing global energy demand pushes the oil industry to target reservoirs with extreme or complicated conditions, such as deep or offshore reservoirs. Conventional equation of state (EoS) with classical mixing rules cannot satisfactorily predict or even correlate the phase equilibrium of those systems. A promising model for such systems is the Cubic-Plus-Association (CPA) EoS, which has been successfully applied to well-defined systems containing associating compounds. In this work, a set of correlations was proposed to calculate the CPA model parameters for the narrow cuts in ill-defined C7+ fractions. The correlations were then combined with either the characterization method of Pedersen et al. or that of Whitson et al. to extend CPA to reservoir fluids in presence of water and polar chemical. Such as methanol and monoethylene glycol. With a minimum number of adjustable parameters from binary pairs, satisfactory results have been obtained for different types of phase equilibria in reservoir fluid systems and several relevant model multicomponent systems. In addition, modeling of Mutual solubility between light hydrocarbons and water is also addressed.
The chilled ammonia process absorbs the CO2 at low temperature (2-10 degrees C). The heat of absorption of carbon dioxide by ammonia is significantly lower than for amines. In addition, degradation problems can be avoided and a high carbon dioxide capacity is achieved. Hence, this process shows good perspectives for decreasing the energy requirement. However, a scientific understanding of the processes is required. The properties of the NH3-CO2-H2O system were described using the Extended UNIQUAC electrolyte model developed by Thomsen and Rasmussen in a temperature range from 0 to 110 degrees C and pressure up to 100 bars [1]. The results show that solid phases consisting of ammonium carbonate and bicarbonate are formed in the absorber. The energy requirements in the absorber and in the desorber have been studied. The enthalpy calculations show that an energy requirement for the desorber lower than 2 GJ/ton CO2 can be reached. (c) 2008 Elsevier Ltd. All rights reserved.
CO2 Capture from Flue Gas using Amino Acid Salt Solutions

The reversible absorption of CO2 into a chemical solvent is currently the leading CO2 capture technology. Available solvents are almost exclusively based on aqueous alkanolamine solutions, which entail both economic and environmental complications, making the commercialization of the technology difficult. Amino acid salt solutions have emerged as an alternative to the alkanolamine solutions. A number of advantages make amino acid salt solutions attractive solvents for CO2 capture from flue gas. In the present study CO2 absorption in aqueous solutions of 0.5 M potassium glycinate and 0.5 M monoethanolamine (MEA) were performed, using a stirred cell reactor experimental setup. The absorption of gas containing 10 mol % CO2 and 90 mol % N2 was followed by measuring the percentage of CO2 in the outlet gas. Also the temperature and pH in the solutions were measured during the absorption. The results showed that the CO2 absorption curves of potassium glycinate and MEA are very similar indicating a potential for potassium glycinate as replacement for MEA in chemical absorption of CO2 from flue gas. For both the potassium glycinate and the MEA solutions the CO2 loading capacity was 0.8 mol CO2/mol amine and the pH dropped between 2 and 3 units during the absorption process. In both types of solutions the temperature increased as a result of the CO2 absorption, which is expected due to the exothermic nature of the absorption reaction. The increase in temperature for the potassium glycinate was lower than for MEA indicating a lower heat of absorption/desorption.
Energy Demand for CO2 Solvent Regeneration

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Fosbøl, P. L. (Intern), Thomsen, K. (Intern), Stenby, E. H. (Intern)
Pages: 242-252
Publication date: 2009

Extended UNIQUAC model for thermodynamic modeling of CO2 absorption in aqueous alkanolamine solutions

The extended UNIQUAC model [K. Thomsen, R Rasmussen, Chem. Eng. Sci. 54 (1999) 1787-1802] was applied to the thermodynamic representation of carbon dioxide absorption in aqueous monoethanolamine (MEA), methyl diethanolamine (MDEA) and varied strength mixtures of the two alkanolamines (MEA-MDEA). For these systems, altogether 13 interaction model parameters are adjusted. Out of these parameters, 11 are temperature dependent. All the essential parameters of the model are simultaneously regressed to a collective set of data on the single MEA and MDEA systems. Different types of data are used for modeling and they cover a very wide range of conditions. Vapor-liquid equilibrium (VLE) data for the aqueous alkanolamine systems containing CO2 in the pressure range of 3-13,000 kPa and temperatures of 25-200 C are used. The model is also regressed with the VLE and freezing point depression data of the binary aqueous alkanolamine systems (MEA-water and MDEA-water). The two just mentioned types of data cover the full concentration range of alkanolamines from extremely dilute to almost pure. The experimental freezing point depression data down to the temperature of 20 degrees C are used. Experimental excess enthalpy (H-E) data of the binary MEA-water and MDEA-water systems at 25, 40, 65 and 69 degrees C are used as well. In order to enhance the calculation of the infinite dilution activity coefficients of MEA and MDEA, the pure alkanolamines vapor pressure data in a relevant temperature range (up to almost 230 degrees C) are included in the parameter estimation process. The previously unavailable standard state properties of the alkanolamine ions appearing in this work, i.e. MEA protonate, MEA carbamate and MDEA protonate are determined. The concentration of the species in both MEA and MDEA solutions containing CO2 are predicted by the model and in the case of MEA compared to NMR spectroscopic data.
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Scopus rating (2016): CiteScore 2.33 SJR 0.869 SNIP 1.155
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.874 SNIP 0.998 CiteScore 1.99
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 0.982 SNIP 1.248 CiteScore 2.28
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.007 SNIP 1.274 CiteScore 2.31
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.152 SNIP 1.286 CiteScore 2.31
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.034 SNIP 1.234 CiteScore 2.26
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 0.986 SNIP 1.317
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.133 SNIP 1.164
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.227 SNIP 1.09
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.031 SNIP 1.151
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.034 SNIP 1.245
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.009 SNIP 1.3
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 0.985 SNIP 1.349
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 1.193 SNIP 1.301
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 0.722 SNIP 1.101
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 0.966 SNIP 1.284
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 0.87 SNIP 0.898
Web of Science (2000): Indexed yes
Scopus rating (1999): SJR 0.938 SNIP 0.885
Original language: English
DOIs:
10.1016/j.fluid.2009.05.002
Source: orbit
Source-ID: 247533
Publication: Research - peer-review › Journal article – Annual report year: 2009
Hydrodynamic impact of particle shape in slurry packed liquid chromatography columns

We report on a series of flow velocity and efficiency profiles, which were measured across the cross section of preparative chromatographic columns packed with different stationary phase materials using computed tomography. It is shown that this non-invasive technique is very useful for visualization of the inner part of a packed column and measurement of the spatial resolved column packing properties. For evaluation of the influence of the particle shape on the velocity distribution and column performance, irregular and spherical reversed phases were studied in detail. The results showed a decreasing velocity towards the column wall most certainly due to a lower permeability. This effect was much less pronounced in the case of spherical particles, indicating a more homogenous packing structure. The influence of the column packing pressure, as a possible measure for improvement of the packing homogeneity was also studied. It was shown that under the same packing conditions spherical particles always lead to a more homogeneous packing. The overall results of this work contribute to the origin of the fact that spherical material is superior to irregular one from the hydrodynamic point of view.

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering
Authors: Lottes, F. (Ekstern), Arlt, W. (Ekstern), Minceva, M. (Ekstern), Stenby, E. H. (Intern)
Pages: 5687-5695
Publication date: 2009
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Chromatography A
Volume: 1216
Issue number: 30
ISSN (Print): 0021-9673
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.97 SJR 1.462 SNIP 1.295
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.713 SNIP 1.395 CiteScore 4.03
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.825 SNIP 1.509 CiteScore 4.28
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 2.017 SNIP 1.616 CiteScore 4.6
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 2.31 SNIP 1.703 CiteScore 4.6
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 2.433 SNIP 1.663 CiteScore 4.47
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 2.207 SNIP 1.566
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 2.136 SNIP 1.571
Improving Mechanistic CO2 Corrosion Models

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Fosbøl, P. L. (Intern), Thomsen, K. (Intern), Stenby, E. H. (Intern)
Publication date: 2009

Host publication information
Title of host publication: Proceedings CORROSION/09
Volume: Paper no. 09561
Publisher: National Association of Corrosion Engineers
Main Research Area: Technical/natural sciences
Conference: CORROSION 2009 : NACE Conference, Atlanta, Georgia, USA, 01/01/2009
Source: orbit
Source-ID: 239780
Publication: Research - peer-review › Article in proceedings – Annual report year: 2009

Mathematical Model for Microbial Enhanced Oil Recovery with Surfactant Distributed between Phases

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering
Authors: Nielsen, S. M. (Intern), Shapiro, A. (Intern), Michelsen, M. L. (Intern), Stenby, E. H. (Intern)
Publication date: 2009

Host publication information
Title of host publication: 30th IEA-EOR Conference
Main Research Area: Technical/natural sciences
Conference: 30th IEA-EOR Conference, Canberra, Australia, 01/01/2009
Measurements and Modelling of CO2 Solubility in Brine and CO2-Saturated Brine Densities at High Pressures

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering
Authors: Yan, W. (Intern), Huang, S. (Ekstern), Stenby, E. H. (Intern)
Publication date: 2009
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 255939
Publication: Research › Poster – Annual report year: 2009

Modeling of the Mixed Solvent Electrolyte System CO2-Na2CO3-NaHCO3-Monoethylene Glycol-Water
The extended UNIQUAC electrolyte activity coefficient model has been correlated to 751 experimental solid−liquid equilibrium (SLE), vapor−liquid equilibrium (VLE), and excess enthalpy data for the mixed solvent CO2−NaHCO3−Na2CO3−monoethylene glycol(MEG)−H2O electrolyte system. The model was validated by predicting the excess heat capacity. The model is consistent, and one set of binary interaction parameters are used for calculating all the properties between −50 and 90 °C. The model is compared to experimental data of infinite dilution activity coefficient measurements of MEG and may be used for calculating activities, solubility, salt hydrate properties, pH, and CO2 solubility in the NaHCO3−Na2CO3−MEG−H2O system. A simple density model of NaHCO3−Na2CO3−NaCl−MEG−water is given.

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Fosbøl, P. L. (Intern), Thomsen, K. (Intern), Stenby, E. H. (Intern)
Pages: 4565-4578
Publication date: 2009
Main Research Area: Technical/natural sciences

Publication information
Journal: Industrial & Engineering Chemistry Research
Volume: 48
Issue number: 9
ISSN (Print): 0888-5885
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.1 SJR 0.945 SNIP 1.139
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.949 SNIP 1.146 CiteScore 2.87
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.012 SNIP 1.292 CiteScore 2.85
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 0.982 SNIP 1.243 CiteScore 2.6
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Phase Identification and Saturation Determination in Carbon Dioxide Flooding of Water Flooded Chalk Using X-Ray Computed Tomography

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering
Authors: Niu, B. (Intern), Yan, W. (Intern), Shapiro, A. (Intern), Stenby, E. H. (Intern)
Publication date: 2009

Host publication information
Title of host publication: IEA EOR Workshop and Symposium 2009
Main Research Area: Technical/natural sciences
Conference: IEA EOR Workshop and Symposium 2009, Canberra, Australia, 01/01/2009
Source: orbit
Source-ID: 265667
Publication: Research - peer-review › Article in proceedings – Annual report year: 2009
Phase Identification and Saturation Determination in Carbon Dioxide Flooding of Water Flooded Chalk Using X-Ray Computed Tomography

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering
Authors: Niu, B. (Intern), Yan, W. (Intern), Shapiro, A. (Intern), Stenby, E. H. (Intern)
Publication date: 2009

Host publication information
Title of host publication: Proceeding from International Symposium of the Society of Core Analysists
Main Research Area: Technical/natural sciences
Conference: International Symposium of the Society of Core Analysists, Noordwijl aan Zee, The Netherlands, 01/01/2009
Source: orbit
Source-ID: 255935
Publication: Research - peer-review › Article in proceedings – Annual report year: 2009

Recent Developments of the CPA equation of state for associating fluids

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering
Authors: Kontogeorgis, G. (Intern), Tsivintzelis, I. (Intern), Breil, M. P. (Intern), Tybjerg, P. C. V. (Ekstern), Stenby, E. H. (Intern), Michelsen, M. L. (Intern)
Number of pages: 74
Publication date: 2009

Host publication information
Title of host publication: Book of Abstracts: 24th ESAT
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 256108
Publication: Research - peer-review › Article in proceedings – Annual report year: 2009

Reverse Schreinemakers Method for Experimental Analysis of Mixed-Solvent Electrolyte Systems
A method based on Schreinemakers's tie-line theory of 1893 is derived for determining the composition and phase amounts in solubility experiments for multi-solvent electrolyte systems. The method uses the lever rule in reverse compared to Schreinemakers's wet residue method, and is therefore called the reverse Schreinemakers (RS) method. The method is based on simple mass balance principles similar to the wet residues method. It allows for accurate determination of the mixed-solvent phase composition even though part of the solvent may precipitate as complexes between solvent and salt. Discrepancies from determining the composition of salt mixtures by pH titration are discussed, and the derived method significantly improves the obtained result from titration. Furthermore, the method reduces the required experimental work needed for analysis of phase composition. The method is applicable to multi-solvent systems and may be used for the determination of solid-phase compositions, similar to Schreinemakers's original "rest" method. An example calculation is presented for the Na2CO3-NaHCO3-MEG-H2O system.

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering
Authors: Fosbøl, P. L. (Intern), Thomsen, K. (Intern), Stenby, E. H. (Intern)
Pages: 1-14
Publication date: 2009
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Solution Chemistry
Volume: 38
Issue number: 1
ISSN (Print): 0095-9782

Ratings:

BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.31 SJR 0.441 SNIP 0.606
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.426 SNIP 0.717 CiteScore 1.26
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.493 SNIP 0.896 CiteScore 1.28
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.485 SNIP 0.805 CiteScore 1.25
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.505 SNIP 0.815 CiteScore 1.25
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.439 SNIP 0.838 CiteScore 1.31
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.559 SNIP 0.809
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.914 SNIP 1.05
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.833 SNIP 0.84
Scopus rating (2007): SJR 0.715 SNIP 0.893
Scopus rating (2006): SJR 0.62 SNIP 0.857
Scopus rating (2005): SJR 0.53 SNIP 0.919
Scopus rating (2004): SJR 0.681 SNIP 1.088
Scopus rating (2003): SJR 0.565 SNIP 1.023
Scopus rating (2002): SJR 0.555 SNIP 0.929
Scopus rating (2001): SJR 0.572 SNIP 0.988
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 0.578 SNIP 1.139
Scopus rating (1999): SJR 0.593 SNIP 0.97

Original language: English

Analysis of mixed-solvent electrolyte solutions, Equilibrium, Schreinemakers's method, Method of wet residue, Analysis of solubility, Restmethode

DOIs:
10.1007/s10953-008-9353-4

Source: orbit
Source-ID: 235636
Publication: Research - peer-review › Journal article – Annual report year: 2009

Simulation of Subsurface Two-Phase Flow in an Oil Reservoir

General information

State: Published
Organisations: Scientific Computing, Department of Informatics and Mathematical Modeling, Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering
Authors: Völcker, C. (Intern), Jørgensen, J. B. (Intern), Thomsen, P. G. (Intern), Stenby, E. H. (Intern)
**Simulation of Two-Phase Flow in an Oil Reservoir using Adaptive High-Order Runge-Kutta based Time-Integration**

**General information**
State: Published  
Organisations: Scientific Computing, Department of Informatics and Mathematical Modeling, Department of Chemistry, Center for Energy Resources Engineering  
Authors: Völcker, C. (Intern), Jørgensen, J. B. (Intern), Thomsen, P. G. (Intern), Stenby, E. H. (Intern)  
Publication date: 2009  
Main Research Area: Technical/natural sciences  
Electronic versions:  
abstract_submit_npcw09.pdf  
Source: orbit  
Source-ID: 268282  
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2009

**Solubility Measurements in the Mixed Solvent Electrolyte System Na2CO3-NaHCO3-Monoethylene Glycol-Water**

**General information**
State: Published  
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering  
Authors: Fosbøl, P. L. (Intern), Thomsen, K. (Intern), Stenby, E. H. (Intern)  
Pages: 2218-2228  
Publication date: 2009  
Main Research Area: Technical/natural sciences

**Publication information**
Journal: Industrial & Engineering Chemistry Research  
Volume: 48  
Issue number: 4  
ISSN (Print): 0888-5885  
Ratings:  
BFI (2018): BFI-level 2  
Web of Science (2018): Indexed yes  
BFI (2017): BFI-level 2  
Web of Science (2017): Indexed yes  
BFI (2016): BFI-level 2  
Scopus rating (2016): CiteScore 3.1 SJR 0.945 SNIP 1.139  
Web of Science (2016): Indexed yes  
BFI (2015): BFI-level 2  
Scopus rating (2015): SJR 0.949 SNIP 1.146 CiteScore 2.87  
Web of Science (2015): Indexed yes  
BFI (2014): BFI-level 2  
Scopus rating (2014): SJR 1.012 SNIP 1.292 CiteScore 2.85  
Web of Science (2014): Indexed yes  
BFI (2013): BFI-level 2  
Scopus rating (2013): SJR 0.982 SNIP 1.243 CiteScore 2.6  
ISI indexed (2013): ISI indexed yes
The Chilled Ammonia Process (CAP) - Energy Requirements by Thermodynamic Modeling

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering
Authors: Fosbøl, P. L. (Intern), Thomsen, K. (Intern), Stenby, E. H. (Intern)
Number of pages: 109
Publication date: 2009

Host publication information
Title of host publication: Book of abstracts: 24th ESAT
Main Research Area: Technical/natural sciences

Original language: English
DOIs: 10.1021/ie8011648
Source: orbit
Source-ID: 239558
Publication: Research - peer-review › Journal article – Annual report year: 2009
The Effects of Possible Contamination on the Radiocarbon Dating of the Dead Sea Scrolls II: Empirical Methods to Remove Castor Oil and Suggestions for Redating

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering, University of Southern Denmark
Authors: Rasmussen, K. L. (Ekstern), van der Plicht, J. (Ekstern), Doudna, G. (Ekstern), Nielsen, F. (Ekstern), Højrup, P. (Ekstern), Stenby, E. H. (Intern), Pedersen, C. T. (Ekstern)
Pages: 1005-1022
Publication date: 2009
Main Research Area: Technical/natural sciences

Publication information
Journal: Radiocarbon
Volume: 51
Issue number: 3
ISSN (Print): 0033-8222
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 4.101 SNIP 2.736 CiteScore 4.53
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 3.425 SNIP 2.377 CiteScore 3.8
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.497 SNIP 1.464 CiteScore 1.97
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.808 SNIP 1.342 CiteScore 1.74
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 4.032 SNIP 2.679 CiteScore 3.93
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 3.14 SNIP 1.89 CiteScore 2.7
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.601 SNIP 1.877
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.878 SNIP 1.038
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.373 SNIP 0.459
Scopus rating (2007): SJR 3.167 SNIP 2.998
Scopus rating (2006): SJR 2.644 SNIP 1.909
Scopus rating (2005): SJR 0.534 SNIP 0.941
Scopus rating (2004): SJR 1.332 SNIP 2.135
Scopus rating (2003): SJR 0.515 SNIP 0.537
Scopus rating (2002): SJR 0.713 SNIP 0.672
Scopus rating (2001): SJR 3.612 SNIP 3.057
Scopus rating (2000): SJR 3.309 SNIP 2.069
The Influence of CO2 Solubility in Brine on CO2 Flooding Simulation

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering
Authors: Yan, W. (Intern), Stenby, E. H. (Intern)
Publication date: 2009

Host publication information
Title of host publication: SPE
Volume: 124628
Main Research Area: Technical/natural sciences
Conference: 2009 SPE ATCE, New Orleans, LA, USA, 01/01/2009
Source: orbit
Source-ID: 255936
Publication: Research › Article in proceedings – Annual report year: 2009

Thermodynamic modeling of the solubility of CO2 in aqueous alkanolamine solutions using the extended UNIQUAC model

Application to monoethanolamine and methyldiethanolamine

The extended UNIQUAC model as proposed by Thomsen and Rasmussen [K. Thomsen, P. Rasmussen, Chem. Eng. Sci. 54 (1999) 1787-1802] was applied to the thermodynamic representation of carbon dioxide absorption in aqueous monoethanolamine (MEA) and methyldiethanolamine (MDEA) solutions. All the essential parameters of the model are simultaneously regressed to a set of data on the MEA and MDEA systems. Freezing point depression, vapor liquid equilibrium (VLE) and excess enthalpy (H-E) data of the binary systems of MEA-water and MDEA-water, VLE data on the ternary CO2-MEA-water as well as CO2-MDEA-water systems in a wide range of temperature (-20-200 degrees C) were used. The application of the model to a large number of experimental data for representation of total pressure over the absorbent solutions (25-200 degrees C), correlation of the excess enthalpy and freezing point depression of the binary solutions of alkanolamine and water and also calculation of pure alkanolamine vapor pressure has been performed with good precision. (C) 2008 Elsevier Ltd. All rights reserved.

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering
Authors: Faramarzi, L. (Intern), Kontogeorgis, G. (Intern), Thomsen, K. (Intern), Stenby, E. H. (Intern)
Pages: 861-867
Publication date: 2009
Main Research Area: Technical/natural sciences

Publication information
Journal: GREENHOUSE GAS CONTROL TECHNOLOGIES 9
Volume: 1
Issue number: 1
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
Thermodynamic Modeling of Water-Acid Gases-Alkanolamine Systems

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Sadegh, N. (Intern), Thomsen, K. (Intern), Stenby, E. H. (Intern), Kontogeorgis, G. (Intern)
Publication date: 2009

Host publication information
Title of host publication: AIChE Annual Meeting
Volume: CD
ISBN (Print): 978-0-8169-1058-6
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 255352
Publication: Research - peer-review › Article in proceedings – Annual report year: 2009

Thermodynamics of Irreversible Processes Enhanced by Mixed Solvent Electrolyte Activity Coefficient Models

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Fosbøl, P. L. (Intern), Thomsen, K. (Intern), Stenby, E. H. (Intern)
Publication date: 2009

Host publication information
Title of host publication: JETC10
Main Research Area: Technical/natural sciences
Conference: Joint European Thermodynamics Conference , Copenhagen, Denmark, 22/06/2009 - 22/06/2009
Source: orbit
Source-ID: 255514
Publication: Research - peer-review › Article in proceedings – Annual report year: 2009

Using Fundamental Advanced Thermodynamics to Model CO2 Capture Using Aqueous Ammonia

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Phase Equilibria and Separation Processes
Using Fundamental Advanced Thermodynamics to understand a CO2 Capture Process

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering
Authors: Darde, V. C. A. (Intern), Thomsen, K. (Intern), van Well, W. J. (Ekstern), Stenby, E. H. (Intern)
Publication date: 2009

Host publication information
Title of host publication: SIMS50
Main Research Area: Technical/natural sciences
Conference: 50th International Conference of Scandinavian Simulation Society, Fredericia, Denmark, 07/10/2009 - 07/10/2009
Source: orbit
Source-ID: 255481
Publication: Research - peer-review › Article in proceedings – Annual report year: 2009

Development of soft nanocarriers from novel amphiphilic hyaluronic acid derivatives towards drug delivery

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering
Authors: Eenschooten, C. D. (Intern), Kontogeorgis, G. (Intern), Stenby, E. H. (Intern), Longin, F. (Ekstern), Schwach-Abdellaoui, K. (Ekstern), Delie, F. (Ekstern), Gurny, R. (Ekstern)
Number of pages: 227
Publication date: Nov 2008

Publication information
ISBN (Print): 978-87-91435-84-6
Original language: English
Main Research Area: Technical/natural sciences
Electronic versions:
Corinne Eenschooten2008.pdf
Source: orbit
Source-ID: 232946
Publication: Research › Ph.D. thesis – Annual report year: 2008

Development of Models and Algorithms for the Study of Reactive Porous Media Processes

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Scientific Computing, Department of Informatics and Mathematical Modeling
Authors: Kristensen, M. R. (Intern), Thomsen, P. G. (Intern), Michelsen, M. L. (Intern), Stenby, E. H. (Intern)
Number of pages: 157
Publication date: May 2008
Statistical methods for history matching


General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Phase Equilibria and Separation Processes
Authors: Johansen, K. (Intern), Shapiro, A. (Intern), Stenby, E. H. (Intern)
Number of pages: 198
Publication date: May 2008

Publication information
Publisher: FRYDENBERG A/S
ISBN (Print): 978-87-91435-75-7
Original language: English
Main Research Area: Technical/natural sciences
Electronic versions:
PhD_Kent_Johansen.pdf
Source: orbit
Source-ID: 222126
Publication: Research › Ph.D. thesis – Annual report year: 2008

Carbon Dioxide Corrosion: Modelling and Experimental Work Applied to Natural Gas Pipelines
CO2 corrosion is a general problem in the industry and it is expensive. The focus of this study is an oil gas production related problem. CO2 corrosion is observed in offshore natural gas transportation pipelines. A general overview of the problem is presented in chapter 1. The chemical system consists mainly of CO2-Na2CO3-NaHCO3-MEG-H2O. Sodium is injected in the pipelines as NaOH in order to pH-stabilize the pipeline to avoid corrosion and MEG is injected in order to prevent gas hydrates. There are a great number of models available in the literature which may predict CO2 corrosion. These models are not very accurate and assume ideality in the main part of the equation. This thesis deals with aspect of improving the models to account for the non-ideality. A general overview and extension of the theory behind electrochemical corrosion is presented in Chapter 2 to 4. The theory deals with the basic thermodynamics of electrolytes in chapter 2, the extension and general description of electrolyte mass transport in chapter 3, and the electrochemical kinetics of corrosion in chapter 4. A literature overview of CO2 corrosion is shown in chapter 5 and possible extensions of the models are discussed. A list of literature cites is given in chapter 6. The literature review in chapter 5 shows how FeCO3 plays a main part in the protection of steel. Especially the solubility of FeCO3 is an important factor. Chapter 7 discusses and validates the thermodynamic properties of FeCO3. The study shows that there is a discrepancy in the properties of FeCO3. Sets of consistent thermodynamic properties of FeCO3 are given. A mixed solvent electrolyte model is regressed in chapter 8 for the CO2-Na2CO3-NaHCO3-MEG-H2O system. Parameters of the extended UNIQUAC model is fitted to literature data of VLE, SLE, heat excess and validated against heat capacity data. The model is also fitted to experimental data produced and shown in chapter 8 for SLE in the Na2CO3-NaHCO3-MEG-H2O system.
application of the above model is shown in chapter 9. Here the thermodynamic correction factors are calculated. These show how the diffusion process in CO2 corrosion models deviate from the ideal case. Conclusion and suggestion for future work are presented in chapter 10 and 11.

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering
Authors: Fosbøl, P. L. (Intern), Stenby, E. H. (Intern), Thomsen, K. (Intern)
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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 Ressources Engineering, Department of Chemistry
Publication date: 2008
Event: Poster session presented at DTU Energy Conference, Technical University of Denmark, Copenhagen, DK.
Main Research Area: Technical/natural sciences
Electronic versions:
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Source: orbit
Source-ID: 232201
Publication: Research - peer-review › Poster – Annual report year: 2008

Chilled ammonia process for CO2 capture

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Darde, V. C. A. (Intern), Thomsen, K. (Intern), Stenby, E. H. (Intern)
Publication date: 2008

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
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CO2 - en drivhusgas og et korrosionsproblem

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering
Authors: Fosbøl, P. L. (Intern), Thomsen, K. (Intern), Stenby, E. H. (Intern)
Pages: 19-22
Hydrolysis of Cellulose Using Mono-Component Enzymes Shows Synergy during Hydrolysis of Phosphoric Acid Swollen Cellulose (PASC), but Competition on Avicel

To study the synergy between the three groups of cellulolytic enzymes, 20 mixtures of different mole percentage of Humicola insolens Cel45A (EG V) and Cel6A (CBH II), and Penicillium brasilianuin Cel3A (O-glucosidase) were used to hydrolyze Avicel and phosphoric acid swollen cellulose/Avicel (PASC). In contrast to previous studies, where P-glucosidase was either not added or added in excess, we here focus on engineering binary, as well as, ternary cellulase mixtures (including a range of different mol% of Cel3A) for maximal total sugar production. Precise hydrolysis pattern based on the concentration of soluble hydrolysis products (glucose to cellohexaose measured by HPLC) was determined. The importance of proper assay selection for hydrolysis products detection was illustrated. It was found that degree of synergy (DS) for degradation of PASC were generally larger than 1 (indicating cooperativity between the enzymes), increasing as the hydrolysis proceeded. DS of binary exo-/endo-glucanase mixtures, decreased as the mol% of Cel45A increased. In contrast to hydrolysis of PASC, DS values during degradation of Avicel were less then 1, indicating inhibition of the involved enzymes. Thus, our data point to competition for the same binding sites between endo- and exo-glucanases, and preferential absorbance of exo-glucanases on crystalline substrates. (c) 2007 Elsevier Inc. All rights reserved.
Phase Equilibria and CO2 Corrosion - A new approach to corrosion modelling

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering
Authors: Fosbøl, P. L. (Intern), Thomsen, K. (Intern), Stenby, E. H. (Intern)
Publication date: 2008
Event: Poster session presented at SPE meeting, Copenhagen, Denmark.
Main Research Area: Technical/natural sciences

The chilled ammonia process - Evaluation of the energy requirements

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Fosbøl, P. L. (Intern), Stenby, E. H. (Intern), Thomsen, K. (Intern)
Publication date: 2008

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 220648
Publication: Research - peer-review › Report – Annual report year: 2008

The Influence of CO2 Solubility in Brine on CO2 Flooding Simulation

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Yan, W. (Intern), Stenby, E. H. (Intern)
Publication date: 2008

Host publication information
Title of host publication: 29th IEA Workshop and Symposium 2008
Main Research Area: Technical/natural sciences
Conference: IEA Workshop and Symposium Collaborative Project on Enhanced Oil Recovery, Beijing, China, 01/01/2008
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Source-ID: 236537
Publication: Research - peer-review › Article in proceedings – Annual report year: 2008

Enzymatic Hydrolysis of Cellulose: Experimental and Modeling Studies

General information
State: Published
Organisations: Center for Microbial Biotechnology, Department of Systems Biology, Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering
Authors: Andersen, N. (Intern), Stenby, E. H. (Intern), Michelsen, M. L. (Intern)
Publication date: Oct 2007

Publication information
Original language: English
CO2 Capture from Coal Fired Power Plants

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering
Authors: Gabrielsen, J. (Intern), Stenby, E. H. (Intern), Michelsen, M. L. (Intern), Kontogeorgis, G. (Intern)
Number of pages: 124
Publication date: Feb 2007

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Electronic versions:
C:\Documents and Settings\alb\Desktop\Ph.D. Jostein Gabrielsen.pdf
Source: orbit
Source-ID: 196087
Publication: Research › Ph.D. thesis – Annual report year: 2007

Modeling of Complex Mixtures Containing Hydrogen Bonding Molecules

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering
Authors: Folas, G. (Intern), Kontogeorgis, G. (Intern), Stenby, E. H. (Intern), Michelsen, M. L. (Intern)
Publication date: Jan 2007

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Electronic versions:
C\Documents_and_Settings\alb\Desktop\Ph.D. Georgios_K._Folas.pdf.pdf
Source: orbit
Source-ID: 196086
Publication: Research › Ph.D. thesis – Annual report year: 2007

An Overview of IVC-SEP

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering
Authors: Stenby, E. H. (Intern)
Publication date: 2007

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 211213
Publication: Education › Compendium/lecture notes – Annual report year: 2007

CAPE-Open: An International Standard for Process Simulation

General information
CO2 capture and storage

General information
CO2 Capture and Storage

General information
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Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering
Authors: Stenby, E. H. (Intern)
Publication date: 2007

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 211212
Publication: Education › Compendium/lecture notes – Annual report year: 2007

CO2 for EOR - Do's and Don'ts

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering
Authors: Stenby, E. H. (Intern)
Publication date: 2007

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 211214
Publication: Research › Sound/Visual production (digital) – Annual report year: 2007

Coupling Chemical Kinetics and Flashes in Reactive, Thermal and Compositional Reservoir Simulation

Phase changes are known to cause convergence problems for integration of stiff kinetics in thermal and compositional reservoir simulations. We propose an algorithm for detection and location of phase changes based on discrete event system theory. The algorithm provides a robust way for handling the switching of variables and equations required when the number of phases changes. We extend the method to handle full phase equilibrium described by an equation of state. Experiments show that the new algorithm improves the robustness of the integration process near phase boundaries by lowering the number of convergence and error test failures by more than 50% compared to direct integration without the
new algorithm. To facilitate the algorithmic development we construct a virtual kinetic cell model. We use implicit one-step ESDIRK (Explicit Singly Diagonal Implicit Runge-Kutta) methods for integration of the kinetics. The kinetic cell model serves both as a tool for the development and testing of tailored solvers as well as a testbed for studying the interactions between chemical kinetics and phase behavior. A comparison between a K-value correlation based approach and a more rigorous equation of state based approach to phase equilibrium shows that phase behavior may significantly impact the reaction paths.

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Kristensen, M. R. (Intern), Gerritsen, M. G. (Ekstern), Thomsen, P. G. (Intern), Michelsen, M. L. (Intern), Stenby, E. H. (Intern)
Number of pages: 12
Pages: 106218-MS
Publication date: 2007

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Title of host publication: SPE Reservoir Simulation Symposium
Main Research Area: Technical/natural sciences
Conference: SPE Reservoir Simulation Symposium, Houston, Texas, USA, 01/01/2007
DOIs: 10.2118/106218-MS
Source: orbit
Source-ID: 211112
Publication: Research - peer-review › Article in proceedings – Annual report year: 2007

Denmark as an Oil Nation

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering
Authors: Stenby, E. H. (Intern)
Publication date: 2007

Publication information
Original language: Danish
Main Research Area: Technical/natural sciences
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Source-ID: 211210
Publication: Research › Sound/Visual production (digital) – Annual report year: 2007

Designing with CAPE-OPEN

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering
Authors: Breil, M. P. (Intern), Gabrielsen, J. (Intern), von Solms, N. (Intern), Kontogeorgis, G. (Intern), Stenby, E. H. (Intern)
Publication date: 2007

Host publication information
Title of host publication: ECCE6
Main Research Area: Technical/natural sciences
Conference: European Congress of Chemical Engineering - 6, Copenhagen, Denmark, 16/09/2007 - 16/09/2007
Source: orbit
Source-ID: 210860
Publication: Research - peer-review › Article in proceedings – Annual report year: 2007

Development of Colloidal Carriers from a Novel Amphiphilic Hyaluronic Acid

General information
Development of Colloidal Carriers from Modified Hyaluronic Acid

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering
Publication date: 2007
Event: Poster session presented at 8th Annual Meeting of the Skin Forum, School of Pharmacy, University of London, London, UK,
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 211264
Publication: Research › Poster – Annual report year: 2007

Diffusion measurements in binary liquid mixtures by Raman spectroscopy
It is shown that Raman spectroscopy allows determination of the molar fractions in mixtures subjected to molecular diffusion. Spectra of three binary systems, benzene/n-hexane, benzene/cyclohexane, and benzene/acetone, were obtained during vertical (exchange) diffusion at several different heights (z) as a function of time. A procedure to determine time-dependent concentration profiles and diffusion coefficients is described in detail for one system, and results are given for the two other cases. For the system benzene/cyclohexane, much lower diffusion coefficients than reported in the literature were found, even in a thermostatically controlled diffusion cell, recording spectra through circulating water. For the system benzene/acetone, the determined diffusion coefficients were in good agreement with the literature data. The limitations of the Raman method are discussed, and it is concluded that many more systems ought to be studied. It is pointed out that diffusion profiles can be obtained in ternary and higher systems, where proper measurements are almost nonexistent.

General information
State: Published
Organisations: Energy and Materials, Department of Chemistry, Department of Chemical and Biochemical Engineering, Center for Phase Equilibria and Separation Processes, Center for Energy Resources Engineering
Authors: Berg, R. W. (Intern), Hansen, S. B. (Intern), Shapiro, A. (Intern), Stenby, E. H. (Intern)
Pages: 367-373
Diffusionsmålinger med Ramanspektroskopi: Viden om diffusioner er i mange sammenhænge af stor betydning. Her beskrives en simpel måde til at studere diffusioner i væsker

General information
State: Published
Organisations: Department of Chemistry, Energy and Materials, Department of Chemistry, Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering
Authors: Hansen, S. B. (Intern), Berg, R. W. (Intern), Shapiro, A. (Intern), Stenby, E. H. (Intern)
Pages: 33-35
Publication date: 2007
Main Research Area: Technical/natural sciences

Publication information
Journal: Dansk Kemi
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ISI indexed (2013): ISI indexed no
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ISI indexed (2011): ISI indexed no
Web of Science (2007): Indexed yes
Web of Science (2004): Indexed yes
Original language: Danish
Electronic versions:
sus-danskkemi-korrektur.pdf
Links:
http://www.techmedia.dk/default.asp?Action=Details&Item=3126

Bibliographical note
For oplysninger om vore øvrige aktiviteter se hjemmesiderne
Source: orbit
Source-ID: 194308
Publication: Communication › Journal article – Annual report year: 2007

Efficient integration of stiff kinetics with phase change detection for reactive reservoir processes
We propose the use of implicit one-step Explicit Singly Diagonal Implicit Runge-Kutta (ESDIRK) methods for integration of the stiff kinetics in reactive, compositional and thermal processes that are solved using operator-splitting type approaches. To facilitate the algorithmic development we construct a virtual kinetic cell model. The model serves both as a tool for the development and testing of tailored solvers as well as a testbed for studying the interactions between chemical kinetics and phase behavior. As case study, two chemical kinetics models with 6 and 14 components, respectively, are implemented for in situ combustion, a thermal oil recovery process. Through benchmark studies using the 14 component reaction model the new ESDIRK solvers are shown to improve computational speed when compared to the widely used multi-step BDF methods DASSL and LSODE. Phase changes are known to cause convergence problems for the integration method. We propose an algorithm for detection and location of phase changes based on discrete event system theory. Experiments show that the algorithm improves the robustness of the integration process near phase boundaries by lowering the number convergence and error test failures by more than 50% compared to direct integration without the new algorithm.

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Equilibria in the mixed solvent system Glycol-NaOH-CO2-Water applied to corrosion modelling

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Fosbøl, P. L. (Intern), Thomsen, K. (Intern), Stenby, E. H. (Intern)
Number of pages: 137
Publication date: 2007

Experimental investigation of liquid chromatography columns by means of computed tomography
The efficiency of packed chromatographic columns was investigated experimentally by means of computed tomography (CT) techniques. The measurements were carried out by monitoring tracer fronts in situ inside the chromatographic columns. The experimental results were fitted using the equilibrium dispersive model (EDM) and varying the so called apparent axial dispersion coefficient. The additivity of the first and second central moments was exploited to estimate column efficiency in different regions of the column. The results showed that the columns under investigation offered a higher column efficiency in the centre compared to the wall region. Furthermore the void fraction in the vicinity of the walls was lower than that in the column core. For this reason the bands were conveyed faster in the central region of the column where the permeability was higher. This result is in good agreement with earlier findings.

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Pages: 9-19
Publication date: 2007
Main Research Area: Technical/natural sciences

Publication information
Journal: Adsorption
Volume: 13
Issue number: 1
ISSN (Print): 0929-5607
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 0.652 SNIP 1.03 CiteScore 2.19
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.748 SNIP 0.859 CiteScore 1.94
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.645 SNIP 0.861 CiteScore 1.84
BFI (2013): BFI-level 1
Experimental validation of a rate-based model for CO2 capture using an AMP solution

Detailed experimental data, including temperature profiles over the absorber, for a carbon dioxide (CO2) absorber with structured packing in an integrated laboratory pilot plant using an aqueous 2-amino-2-methyl-1-propanol (AMP) solution are presented. The experimental gas-liquid material balance was within an average of 3.5% for the experimental conditions presented. A predictive rate-based steady-state model for CO2 absorption into an AMP solution, using an implicit expression for the enhancement factor, has been validated against the presented pilot plant data. Furthermore, a parameter sensitivity analysis for the proposed model has been carried out.

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Gabrielsen, J. (Intern), Svendsen, H. F. (Ekster), Michelsen, M. L. (Intern), Stenby, E. H. (Intern), Kontogeorgis, G. (Intern)
Pages: 2397-2413
Publication date: 2007
Main Research Area: Technical/natural sciences

Publication information
Journal: Chemical Engineering Science
Volume: 62
Issue number: 9
ISSN (Print): 0009-2509
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2  
Web of Science (2017): Indexed yes  
BFI (2016): BFI-level 2  
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  
DOIs: 
10.1016/j.ces.2007.01.034  
Source: orbit  
Source-ID: 198594  
Publication: Research - peer-review › Journal article – Annual report year: 2007
Fluid characterization for miscible EOR projects and CO2 sequestration

Accurate performance prediction of miscible enhanced-oil-recovery (EOR) projects or CO2 sequestration in depleted oil and gas reservoirs relies in part on the ability of an equation-of-state (EOS) model to adequately represent the properties of a wide range of mixtures of the resident fluid and the injected fluid(s). The mixtures that form when gas displaces oil in a porous medium will, in many cases, differ significantly from compositions created in swelling tests and other standard pressure/volume/temperature (PVT) experiments. Multicontact experiments (e.g., slimtube displacements) are often used to condition an EOS model before application in performance evaluation of miscible displacements. However, no clear understanding exists of the impact on the resultant accuracy of the selected characterization procedure when the fluid description is subsequently included in reservoir simulation. In this paper, we present a detailed analysis of the quality of two different characterization procedures over a broad range of reservoir fluids (13 samples) for which experimental swelling-test and slimtube-displacement data are available. We explore the impact of including swelling-test and slimtube experiments in the data reduction and demonstrate that for some gas/oil systems, swelling tests do not contribute to a more accurate prediction of multicontact miscibility. Finally, we report on the impact that use of EOS models based on different characterization procedures can have on recovery predictions from dynamic ID displacement calculations.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Phase Equilibria and Separation Processes, Center for Energy Resources Engineering
Authors: Jessen, K. (Intern), Stenby, E. H. (Intern)
Pages: 482-488
Publication date: 2007
Main Research Area: Technical/natural sciences

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Journal: SPE Reservoir Evaluation and Engineering
Volume: 10
Issue number: 5
ISSN (Print): 1094-6470
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 0.886 SNIP 1.856 CiteScore 3.37
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.023 SNIP 2.224 CiteScore 2.58
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.835 SNIP 1.833 CiteScore 2.33
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.809 SNIP 1.36 CiteScore 1.91
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.089 SNIP 1.641 CiteScore 1.77
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.339 SNIP 1.79 CiteScore 1.85
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.084 SNIP 1.712
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.736 SNIP 1.118
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.318 SNIP 0.917
Scopus rating (2007): SJR 0.569 SNIP 0.698
Web of Science (2007): Indexed yes
This work presents new experimental phase equilibrium measurements of the binary MEG-methane and the ternary MEG-water-methane system at low temperatures and high pressures which are of interest to applications related to natural gas processing. Emphasis is given to MEG and water solubility measurements in the gas phase. The CPA and SRK EoS, the latter using either conventional or EoS/G(E) mixing rules are used to predict the solubility of the heavy components in the gas phase. It is concluded that CPA and SRK using the Huron-Vidal mixing rule perform equally satisfactory, while CPA requires fewer interaction parameters. (c) 2006 Elsevier B.V. All rights reserved.
How to Collaborate with International Industry on Research and Innovation as Academic Researchers

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering
Authors: Stenby, E. H. (Intern)
Publication date: 2007

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 211216
Publication: Research › peer-review › Journal article – Annual report year: 2007
Modelling of associating mixtures for applications in the oil and gas and chemical industries

Thermodynamic properties and phase equilibria of associating mixtures cannot often be satisfactorily modelled using conventional models such as cubic equations of state. CPA (cubic-plus-association) is an equation of state (EoS), which combines the SRK EoS with the association term of SAFT. For non-polar (non self-associating) compounds it reduces to SRK. The model was first published in 1996 and since then it has been developed and applied with success to binary systems containing water-alkanes and alcohol/glycol/acid-alkanes (both VLE and LLE) as well as ternary and multicomponent (V)LLE for water-alcohol (glycol)-alkanes and certain acid and amine-containing mixtures. Recent results include glycol-aromatic hydrocarbons including multiphase, multicomponent equilibria and gas hydrate calculations in combination with the van der Waals-Platteeuw model. This article will outline some new applications of the model of relevance to the petroleum and chemical industries: high pressure vapor-liquid and liquid-liquid equilibrium in alcohol-containing mixtures, mixtures with gas hydrate inhibitors and mixtures with polar and hydrogen bonding chemicals including organic acids. Some comparisons with conventional thermodynamic models especially those combining cubic
EoS with local composition activity coefficient models are included. (C) 2007 Elsevier B.V. All rights reserved.

**General information**

- **State:** Published
- **Organisations:** Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
- **Authors:** Kontogeorgis, G. (Intern), Folas, G. (Intern), Muro Sunè, N. (Intern), von Solms, N. (Intern), Michelsen, M. L. (Intern), Stenby, E. H. (Intern)
- **Pages:** 205-211
- **Publication date:** 2007
- **Conference:** 11th International Conference on Properties and Phase Equilibria for Product and Process Design Crete, Crete, Greece, 20/05/2007 - 20/05/2007
- **Main Research Area:** Technical/natural sciences

**Publication information**

- **Journal:** Fluid Phase Equilibria
- **Volume:** 261
- **Issue number:** 1-2
- **ISSN (Print):** 0378-3812
- **Ratings:**
  - BFI (2018): BFI-level 2
  - Web of Science (2018): Indexed yes
  - BFI (2017): BFI-level 2
  - Web of Science (2017): Indexed yes
  - BFI (2016): BFI-level 2
  - Scopus rating (2016): CiteScore 2.33 SJR 0.869 SNIP 1.155
  - Web of Science (2016): Indexed yes
  - BFI (2015): BFI-level 2
  - Scopus rating (2015): SJR 0.874 SNIP 0.998 CiteScore 1.99
  - Web of Science (2015): Indexed yes
  - BFI (2014): BFI-level 2
  - Scopus rating (2014): SJR 0.982 SNIP 1.248 CiteScore 2.28
  - Web of Science (2014): Indexed yes
  - BFI (2013): BFI-level 2
  - Scopus rating (2013): SJR 1.007 SNIP 1.274 CiteScore 2.31
  - ISI indexed (2013): ISI indexed yes
  - Web of Science (2013): Indexed yes
  - BFI (2012): BFI-level 2
  - Scopus rating (2012): SJR 1.152 SNIP 1.286 CiteScore 2.31
  - ISI indexed (2012): ISI indexed yes
  - Web of Science (2012): Indexed yes
  - BFI (2011): BFI-level 2
  - Scopus rating (2011): SJR 1.034 SNIP 1.234 CiteScore 2.26
  - ISI indexed (2011): ISI indexed yes
  - Web of Science (2011): Indexed yes
  - BFI (2010): BFI-level 2
  - Scopus rating (2010): SJR 0.986 SNIP 1.317
  - Web of Science (2010): Indexed yes
  - BFI (2009): BFI-level 2
  - Scopus rating (2009): SJR 1.133 SNIP 1.164
  - Web of Science (2009): Indexed yes
  - BFI (2008): BFI-level 1
  - Scopus rating (2008): SJR 1.227 SNIP 1.09
  - Web of Science (2008): Indexed yes
  - Scopus rating (2007): SJR 1.031 SNIP 1.151
  - Web of Science (2007): Indexed yes
  - Scopus rating (2006): SJR 1.034 SNIP 1.245
Modelling of Associating Mixtures for Applications in the Oil and Gas and Chemical Industries

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering
Authors: Kontogeorgis, G. (Intern), Michelsen, M. L. (Intern), Folas, G. (Intern), von Solms, N. (Intern), Stenby, E. H. (Intern)
Publication date: 2007

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 211147
Publication: Research › Sound/Visual production (digital) – Annual report year: 2007

Modelling of CO2 Capture

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering
Authors: Breil, M. P. (Intern), Kontogeorgis, G. (Intern), Stenby, E. H. (Intern)
Publication date: 2007

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 210856
Publication: Research › Sound/Visual production (digital) – Annual report year: 2007

Oil - plenty for this and the next generation

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering
Petroleum Research at DTU - Challenges and Perspectives

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering
Authors: Stenby, E. H. (Intern)
Publication date: 2007

Phase equilibria and CO2 corrosion - A new approach to corrosion modelling

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering
Authors: Fosbøl, P. L. (Intern), Thomsen, K. (Intern), Stenby, E. H. (Intern)
Publication date: 2007
Event: Poster session presented at NACExpo 2007 Conference, Nashville, TN, USA.
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 210957
Publication: Research › Poster – Annual report year: 2007

Phase equilibria and CO2 corrosion - A new approach to corrosion modelling

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering
Authors: Fosbøl, P. L. (Intern), Thomsen, K. (Intern), Stenby, E. H. (Intern)
Publication date: 2007
Event: Poster session presented at Future Energy Research Conference, RISØ, Denmark.
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 210965
Publication: Research › Poster – Annual report year: 2007

Phase equilibria and CO2 corrosion - A new approach to corrosion modelling

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering
Authors: Fosbøl, P. L. (Intern), Thomsen, K. (Intern), Stenby, E. H. (Intern)
Publication date: 2007
Phase equilibria and CO2 corrosion - A new approach to corrosion modelling

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering
Authors: Fosbøl, P. L. (Intern), Thomsen, K. (Intern), Stenby, E. H. (Intern)
Publication date: 2007
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 210959
Publication: Research › Poster – Annual report year: 2007

Recent Results from the Petroleum Engineering Research at IVC-SEP

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering
Authors: Stenby, E. H. (Intern)
Publication date: 2007

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 211211
Publication: Research › Sound/Visual production (digital) – Annual report year: 2007

Solvation Phenomena in Association Theories

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering
Authors: Kontogeorgis, G. (Intern), Folas, G. (Intern), Muro-Sune, N. (Ekstern), Roca Leon, F. (Intern), von Solms, N. (Intern), Michelsen, M. L. (Intern), Stenby, E. H. (Intern)
Publication date: 2007

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 211149
Publication: Research › Sound/Visual production (digital) – Annual report year: 2007

Study of asphaltene precipitation by Calorimetry
Can calorimetry bring new input to the Current understanding of asphaltene precipitation? In this work, two types of precipitation were studied by means of calorimetry: addition of n-heptane into asphaltene solutions and temperature/pressure variations on a recombined live oil. The first series of experiments showed that weak forces determine precipitation. Indeed, isothermal titration calorimetry could not detect any clear signal although this technique can detect low-energy transitions such as liquid-liquid equilibrium and micellization. The second series of tests proved that precipitation caused by T and P variations is exothermic for this system. Furthermore, the temperature-induced precipitation is accompanied by an increase in the apparent thermal expansivity. Therefore, it seems that these two phase transitions exhibit different calorimetric behaviours and they may not be as similar as expected.
Experimental Study and Modelling of Asphaltene Precipitation Caused by Gas Injection

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Phase Equilibria and Separation Processes
Authors: Verdier, S. C. R. (Intern), Stenby, E. H. (Intern), Andersen, S. I. (Intern)
Publication date: Sep 2006

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Electronic versions: Sylvian Verdier.pdf
Source: orbit
Source-ID: 191322
Publication: Research › Ph.D. thesis – Annual report year: 2006

Application of CPA to Reservoir Fluids in Presence of Water and Other Associating Compounds

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering
Authors: Yan, W. (Intern), Kontogeorgis, G. (Intern), Stenby, E. H. (Intern)
Pages: 80-83
Publication date: 2006

Host publication information
Title of host publication: ESAT 2006 22nd European Symposium on Applied Thermodynamics
ISBN (Print): 87-91435-39-0
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 192801
Publication: Research › peer-review › Article in proceedings – Annual report year: 2006

Application of CPA to Reservoir Fluids in Presence of Water and Other Associationg Compounds

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering
Authors: Yan, W. (Intern), Kontogeorgis, G. (Intern), Stenby, E. H. (Intern)
Publication date: 2006
Event: Poster session presented at 22nd European Symposium on Applied Thermodynamic, Elsinore, Denmark.
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 192804
Publication: Research › peer-review › Poster – Annual report year: 2006

Application of the cubic-plus-association (CPA) equation of state to complex mixtures with aromatic hydrocarbons
The cubic-plus-association (CPA) equation of state is applied to phase equilibria of mixtures containing alcohols, glycols, water, and aromatic or olefinic hydrocarbons. Previously, CPA has been successfully used for mixtures containing various associating compounds (alcohols, glycols, amines, organic acids, and water) and aliphatic hydrocarbons. We show in this work that the model can be satisfactorily extended to complex vapor-liquid-liquid equilibria with aromatic or olefinic hydrocarbons. The solvation between aromatics/olefins and polar compounds is accounted for. This is particularly important for mixtures containing water and glycols, but less so for mixtures with alcohols. For water/hydrocarbons, a single binary interaction parameter which accounts for the solvation is fitted to the experimental liquid-liquid equilibria.
(LLE) data. The interaction parameter of the physical term of the model (the Soave-Redlich-Kwong (SRK) equation of state) can be obtained from mixtures with aliphatic hydrocarbons. For mixtures of glycols with aromatic hydrocarbons, two parameters have been fitted to experimental data, one in the physical (SRK) part and one in the association part of the model. Satisfactory liquid-liquid equilibrium predictions are obtained for multicomponent water-alcohol/glycol-aromatic hydrocarbons using solely parameters obtained from binary data.

**General information**

State: Published  
Organisations: Department of Chemical and Biochemical Engineering, Center for Phase Equilibria and Separation Processes, Center for Energy Resources Engineering  
Authors: Folas, G. (Intern), Kontogeorgis, G. (Intern), Michelsen, M. L. (Intern), Stenby, E. H. (Intern)  
Pages: 1527-1538  
Publication date: 2006  
Main Research Area: Technical/natural sciences

**Publication information**

Journal: Industrial & Engineering Chemistry Research  
Volume: 45  
Issue number: 4  
ISSN (Print): 0888-5885  
Ratings:  
BFI (2018): BFI-level 2  
Web of Science (2018): Indexed yes  
BFI (2017): BFI-level 2  
Web of Science (2017): Indexed yes  
BFI (2016): BFI-level 2  
Web of Science (2016): Indexed yes  
BFI (2015): BFI-level 2  
Scopus rating (2016): CiteScore 3.1 SJR 0.945 SNIP 1.139  
Web of Science (2016): Indexed yes  
BFI (2014): BFI-level 2  
Scopus rating (2014): SJR 1.012 SNIP 1.292 CiteScore 2.85  
Web of Science (2014): Indexed yes  
BFI (2013): BFI-level 2  
Scopus rating (2013): SJR 0.982 SNIP 1.243 CiteScore 2.6  
ISI indexed (2013): ISI indexed yes  
Web of Science (2013): Indexed yes  
BFI (2012): BFI-level 2  
Scopus rating (2012): SJR 1.066 SNIP 1.338 CiteScore 2.56  
ISI indexed (2012): ISI indexed yes  
Web of Science (2012): Indexed yes  
BFI (2011): BFI-level 2  
Scopus rating (2011): SJR 1.086 SNIP 1.24 CiteScore 2.58  
ISI indexed (2011): ISI indexed yes  
Web of Science (2011): Indexed yes  
BFI (2010): BFI-level 2  
Scopus rating (2010): SJR 1.047 SNIP 1.165  
Web of Science (2010): Indexed yes  
BFI (2009): BFI-level 2  
Scopus rating (2009): SJR 1.002 SNIP 1.164  
Web of Science (2009): Indexed yes  
BFI (2008): BFI-level 2  
Scopus rating (2008): SJR 1.142 SNIP 1.267  
Web of Science (2008): Indexed yes  
Scopus rating (2007): SJR 1.105 SNIP 1.239  
Web of Science (2007): Indexed yes
Application of the cubic-plus-association equation of state to mixtures with polar chemicals and high pressures

The cubic-plus-association (CPA) equation of state has been previously applied to vapor-liquid, liquid-liquid, and solid-liquid equilibria of mixtures containing associating compounds (water, alcohols, glycols, acids, amines). Although some high-pressure applications have been presented, emphasis was given to low pressures and liquid-liquid equilibria. In this work, CPA is applied to two classes of mixtures containing polar chemicals for which high-pressure data are available: acetone-containing systems and dimethyl ether mixtures. They are of both scientific and industrial importance. Moreover, CPA is applied to high-pressure solid-liquid equilibria (SLE) for alcohol-alkane mixtures. In the case of acetone-hydrocarbon mixtures, satisfactory results are achieved if acetone is allowed to self-associate. Satisfactory high-pressure acetone-water vapor-liquid equilibrium (VLE) is obtained, comparable to conventional models such as MHV2. Very good results are also obtained for multicomponent vapor-liquid-liquid equilibria for mixtures containing gases, water, and dimethyl ether. Finally, it is shown that high-pressure SLE can be predicted based on interaction parameters obtained from low-pressure SLE data.

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Folas, G. (Intern), Kontogeorgis, G. (Intern), Michelsen, M. L. (Intern), Stenby, E. H. (Intern)
Pages: 1516-1526
Publication date: 2006
Main Research Area: Technical/natural sciences

Publication information
Journal: Industrial & Engineering Chemistry Research
Volume: 45
Issue number: 4
ISSN (Print): 0888-5885
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.1 SJR 0.945 SNIP 1.139
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.949 SNIP 1.146 CiteScore 2.87
Asphaltene Precipitation and Calorimetry

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Phase Equilibria and Separation Processes
CO2 udskillelse og lagring - muligheder og udfordringer

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering
Authors: Stenby, E. H. (Intern)
Publication date: 2006

Host publication information
Title of host publication: DK2 - Dansk Kemiingeniør Konference 2006
ISBN (Print): 87-91435-36-6
Main Research Area: Technical/natural sciences
Conference: 2. Dansk Kemiingeniørkonference, Kgs.Lyngby, Denmark, 31/05/2006 - 31/05/2006
Source: orbit
Source-ID: 193115
Publication: Research - peer-review › Article in proceedings – Annual report year: 2006

Corrosion in mixed solvent electrolyte systems

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering
Authors: Fosbøl, P. L. (Intern), Thomsen, K. (Intern), Stenby, E. H. (Intern)
Publication date: 2006
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 193458
Publication: Research - peer-review › Poster – Annual report year: 2006

Efficient Integration of Stiff Kinetics in Reactive Compositional and Thermal Porous Media Processes

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering
Authors: Kristensen, M. R. (Intern), Gerritsen, M. (Ekstern), Thomsen, P. G. (Ekstern), Michelsen, M. L. (Intern), Stenby, E. H. (Intern)
Publication date: 2006

Host publication information
Title of host publication: 10th European Conference on the Mathematics of Oil Recovery (ECMOR)
Main Research Area: Technical/natural sciences
Conference: 10th European Conference on the Mathematics of Oil Recovery (ECMOR), Amsterdam, The Netherlands, September 4-7, 01/01/2006
Source: orbit
Source-ID: 192787
Publication: Research - peer-review › Article in proceedings – Annual report year: 2006

Efficient Reaction Integration for In-Situ Combustion Simulation

General information
Liquid-liquid equilibria for binary and ternary systems containing glycols + aromatic hydrocarbons

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering
Authors: Folas, G. (Intern), Kontogeorgis, G. (Intern), Michelsen, M. L. (Intern), Stenby, E. H. (Intern), Solbraa, E. (Ekstern)
Publication date: 2006
Event: Poster session presented at 22nd European Symposium on Applied Thermodynamic, Elsinore, Denmark.
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 192813
Publication: Research - peer-review › Poster – Annual report year: 2006

Liquid-liquid equilibria for binary and ternary systems containing glycols, aromatic hydrocarbons, and water: Experimental measurements and modeling with the CPA EoS

Liquid-liquid equilibrium data of four binary glycol + aromatic hydrocarbon systems and three ternary systems containing water have been measured at atmospheric pressure. The measured systems are monoethylene glycol (MEG) + benzene or toluene, triethylene glycol (TEG) + benzene or toluene, MEG + water + benzene, MEG + water + toluene, and TEG + water + toluene. The binary systems are correlated with the Cubic-Plus-Association (CPA) equation of state while the ternary systems are predicted from interaction parameters obtained from the binary systems. Very satisfactory liquid-liquid equilibrium correlations are obtained for the binary systems using temperature-independent interaction parameters, while adequate predictions are achieved for multicomponent water + glycol + aromatic hydrocarbons systems when accounting for the solvation between the aromatic hydrocarbons and glycols or water.

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Folas, G. (Intern), Kontogeorgis, G. (Intern), Michelsen, M. L. (Intern), Stenby, E. H. (Intern), Solbraa, E. (Ekstern)
Pages: 977-983
Publication date: 2006
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Chemical and Engineering Data
Volume: 51
Issue number: 3
ISSN (Print): 0021-9568
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.29 SJR 0.88 SNIP 1.097
Web of Science (2016): Indexed yes
Modeling of CO2 absorber using an AMP solution

Abstract: An explicit model for carbon dioxide (CO2) solubility in an aqueous solution of 2-amino-2-methyl-1-propanol (AMP) has been proposed and an expression for the heat of absorption of CO2 has been developed as a function of loading and temperature. A rate-based steady-state model for CO2 absorption into an AMP solution has been proposed, using both the proposed expression for the CO2 solubility and the expression for the heat of absorption along with an expression for the enhancement factor and physicochemical data from the literature. The proposed model has successfully been applied to absorption of CO2 into an AMP solution in a packed tower and validated against pilot-plant
Modeling of Randomly Packed CO2 Absorber Using an Alkanolamine Solution

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering
Authors: Gabrielsen, J. (Intern), Michelsen, M. L. (Intern), Stenby, E. H. (Intern), Kontogeorgis, G. (Intern)
Publication date: 2006
Event: Poster session presented at 22nd European Symposium on Applied Thermodynamic, Elsinore, Denmark.
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 192803
Publication: Research - peer-review › Poster – Annual report year: 2006

Modelling of Randomly Packed CO2 Absorber Using an Alkanolamine Solution

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering
Authors: Gabrielsen, J. (Intern), Michelsen, M. L. (Intern), Stenby, E. H. (Intern), Kontogeorgis, G. (Intern)
Publication date: 2006
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 193120
Publication: Research - peer-review › Poster – Annual report year: 2006

Multicomponent Adsorption Approaches to Modeling Adsorption Equilibria

General information
State: Published
Organisations: CERE – Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Shapiro, A. (Intern), Stenby, E. H. (Intern)
Number of pages: 8,032
Pages: 4180-4189
Publication date: 2006

Host publication information
Title of host publication: Encyclopedia of Surface and Colloid Science
Place of publication: New York
Publisher: C R C Press LLC
**Numerical Simulation of In-Situ Combustion**

**General information**
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering
Authors: Kristensen, M. R. (Intern), Thomsen, P. G. (Ekstern), Michelsen, M. L. (Intern), Stenby, E. H. (Intern)
Publication date: 2006
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 191858
Publication: Research - peer-review › Book chapter – Annual report year: 2006

**On the Process of Gas Liberation in Porous Media**
The aim of the present work is an experimental and computational analysis of the effect of gas liberation in a porous medium. The experiments are based on application of X-ray computed tomography (CT). A series of experiments on slow gas liberation was carried out. A mathematical model of the liberation process was developed based on the theory of differential depletion in the presence of a porous medium. The porous samples involved were low-permeable North Sea core plugs and artificial glass core. The results of the experiments indicate rather uniform gas production in different parts of the samples. The results of the calculations indicate noticeable, although not extreme, lowering of the bubble point pressure (0.12-0.18 MPa) and decreased production of gas, compared to the depletion carried out in a PVT cell.

**General information**
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Phase Equilibria and Separation Processes, Center for Energy Resources Engineering
Authors: Zhelezny, P. (Intern), Shapiro, A. (Intern), Vu, D. T. (Intern), Stenby, E. H. (Intern)
Pages: 503-521
Publication date: 2006
Main Research Area: Technical/natural sciences
Publication information
Journal: Journal of Porous Media
Volume: 9
Issue number: 6
ISSN (Print): 1091-028X
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 0.492 SNIP 0.744 CiteScore 1.22
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.456 SNIP 0.789 CiteScore 1.05
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.365 SNIP 0.654 CiteScore 0.81
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.295 SNIP 0.488 CiteScore 0.6
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.385 SNIP 0.617 CiteScore 0.65
ISI indexed (2012): ISI indexed yes
Pipeline Corrosion - Carbonate Solubility in Mixed Solvent Electrolyte System

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering
Authors: Fosbøl, P. L. (Intern), Stenby, E. H. (Intern), Thomsen, K. (Intern)
Publication date: 2006
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 193110
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2006

Prediction of Gas Phase Water Content of High Pressure Nitrogen, Methane and Natural Gas

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering
Authors: Folas, G. (Intern), Løvland, J. (Ekstern), Kontogeorgis, G. (Intern), Michelsen, M. L. (Intern), Stenby, E. H. (Intern), Solbraa, E. (Ekstern)
Publication date: 2006
Event: Poster session presented at 22nd European Symposium on Applied Thermodynamics, Elsinore, Denmark.
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 192812
Publication: Research - peer-review › Poster – Annual report year: 2006

Prediction of Mineral Scale Formation in Geothermal and Oilfield Operations Using the Extended UNIQUAC Model - Part II. Carbonate-scaling Minerals
Two additional parameters to account for the pressure dependency of solubility are added to the Extended UNIQUAC model presented by Thomsen and Rasmussen (1999). The improved model has been used for correlation and prediction of vapor-liquid-solid equilibrium for different carbonate systems (CaCO3, MgCO3, BaCO3 and SrCO3) causing scale problems. The solubility of NaCl and CO2 in pure water, and the solubility of CO2 in solutions of different salts (NaCl and
Na2SO4) have also been correlated. The temperature and pressure range covered is from 0 to 250°C and from 1 to 1000 bar, respectively. The results show that the Extended UNIQUAC model, with the proposed pressure parameters, is able to represent binary (NaCl-H2O, MCO3-H2O and CO2-H2O), ternary (MCO3-CO2-H2O, CO2-NaCl-H2O and CO2-Na2SO4-H2O) and quaternary (CO2-NaCl-Na2SO4-H2O) solubility data within the experimental accuracy in the temperature range from 0 to 250°C, and the pressure range from 1 to 1000 bar. M stands for Ca2+, Mg2+, Ba2+ and Sr2+.
Prediction of viscosities and surface tensions of fuels using a new corresponding states model
While some properties of diesels are cheap, easy and fast to measure, such as densities, others such as surface tensions and viscosities are expensive and time consuming. A new approach that uses some basic information such as densities to predict viscosities and surface tensions is here proposed using a Corresponding states model previously developed for the accurate estimation of several thermophysical properties of pure and mixed n-alkanes. This approach is tested with good results in five petroleum distillation cuts from crudes of different sources (North Sea, Africa and Middle East). (C) 2005 Elsevier Ltd. All rights reserved.
Statistical Methods for History Matching

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering
Authors: Johansen, K. (Intern), Shapiro, A. (Intern), Stenby, E. H. (Intern)
Publication date: 2006
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 193453
Publication: Research - peer-review › Poster – Annual report year: 2006

Ten years with the CPA (Cubic-Plus-Association) equation of state. Part 1. Pure compounds and self-associating systems

CPA (Cubic-Plus-Association) is an equation of state that is based on a combination of the Soave-Redlich-Kwong (SRK) equation with the association term of the Wertheim theory. The development of CPA started in 1995 as a research project funded by Shell (Amsterdam), and the model was first published in 1996. Since then, it has been successfully applied to a variety of complex phase equilibria, including mixtures containing alcohols, glycols, organic acids, water, and hydrocarbons. Focus has been placed on cases of industrial importance, e.g., systems with gas-hydrate inhibitors (methanol, glycols), glycol regeneration and gas dehydration units, oxygenate additives in gasoline, alcohol separation, etc. This manuscript, which is the first of a series of two papers, offers a review of previous applications and illustrates current focus areas related to the estimation of pure compound parameters, alcohol-hydrocarbon vapor-liquid equilibria (VLE) and solid-liquid equilibria (SLE), as well as aqueous systems. The capabilities and limitations of CPA are discussed and suggestions for extension of the model to systems not covered in this work are provided.

General information
State: Published
Ten years with the CPA (Cubic-Plus-Association) equation of state. Part 2. Cross-associating and multicomponent systems

In this second article of the review on the applications of the CPA (Cubic-Plus-Association) equation of state, the focus is placed on cross-associating systems. Various such mixtures are investigated, including (i) systems with two self-associating compounds (e.g., water-alcohol systems or glycols, mixtures with organic acids, or two alcohols) but also binaries with only one self-associating substance, where solvation is expected (e.g., CO2 or styrene with water). The method of accounting for cross-association (combining rules) and the association scheme of alcohols are investigated. Finally, the manuscript concludes with a summary of current capabilities and limitations of CPA and a list of future challenges.

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Kontogeorgis, G. (Intern), Michelsen, M. L. (Intern), Folas, G. (Intern), Derawi, S. (Intern), von Solms, N. (Intern), Stenby, E. H. (Intern)
Pages: 4869-4878
Publication date: 2006
Main Research Area: Technical/natural sciences

Publication information
Journal: Industrial & Engineering Chemistry Research
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BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.1 SJR 0.945 SNIP 1.139
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.949 SNIP 1.146 CiteScore 2.87
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.012 SNIP 1.292 CiteScore 2.85
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 0.982 SNIP 1.243 CiteScore 2.6
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
Vapor-liquid, liquid-liquid and vapor-liquid-liquid equilibrium of binary and multicomponent systems with MEG modeling with the CPA EoS and an EoS/G(E) model

The cubic-plus-association (CPA) EoS is applied to multicomponent multiphase equilibria of systems containing MEG as a hydrate inhibitor. It is shown that the model provides very satisfactory prediction of the phase behavior for the systems tested. A more conventional engineering model for handling associating and polar molecules, an EoS/G(E) model is also tested, both for binary and multicomponent systems, and compared to the performance of the CPA EoS. It is found that the performance of CPA is overall superior while using fewer interaction parameters than the EoS/G(E) approach. (c) 2006 Elsevier B.V. All rights reserved.
A model for estimating CO2 solubility in aqueous alkanolamines

Partial pressures of carbon dioxide (CO2) over aqueous solutions of monoethanolamine (MEA), diethanolamine (DEA), and N-methyldiethanolamine (MDEA) have been correlated using a simple approach where only one chemical equilibrium reaction is taken into account and assuming ideal gas and ideal liquid properties. The approach combines the Henry's law constant and the chemical reaction equilibrium constant for the formation of carbamate for primary and secondary alkanolamines (MEA, DEA) or bicarbonate for tertiary alkanolamines (MDEA), resulting in an explicit expression for calculating the partial pressure of CO2 over an aqueous alkanolamine solution. Accurate values for the partial pressure of CO2 are obtained for a limited loading, temperature, and pressure range that is useful in modeling CO2 capture from coal-fired power plants. Heat of absorption values derived from the model agree with experimental data from the literature.
Application of Advanced Thermodynamic Models for Complex Fluids and Reservoirs

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Yan, W. (Intern), Kontogeorgis, G. (Intern), Stenby, E. H. (Intern)
Publication date: 2005

Host publication information
Title of host publication: 26th IEA Annual Workshop & Symposium on Enhanced Oil Recovery
Main Research Area: Technical/natural sciences
Conference: IEA Annual Workshop & Symposium on Enhanced Oil Recovery, Japan, 01/01/2005
Source: orbit
Source-ID: 188060
Publication: Research - peer-review › Article in proceedings – Annual report year: 2005

Application of the cubic-plus-association (CPA) equation of state to cross-associating systems

The cubic-plus-association (CPA) equation of state (EoS) is applied, using different combining rules, to vapor-liquid equilibria (VLE) and liquid-liquid equilibria (LLE) of alcohol-water systems. It is demonstrated that the Elliott combining rule (ECR) with a common temperature-independent interaction parameter provides very adequate VLE correlations over extended temperature and pressure ranges, yielding also a very satisfactory description of the azeotropic behavior. LLE of
heavy alcohol-water systems is best described with the CR-1 combining rule and a single interaction parameter. Satisfactory predictions of multicomponent, multiphase equilibria of water-alcohol-alkane systems at various conditions are achieved using solely one interaction parameter per binary. A study of the dominant binary systems for the prediction of the multicomponent systems demonstrates that both the binary alcohol-water and alcohol-hydrocarbon systems are crucial for the prediction of the partition coefficients of alcohols. Finally, the CPA EoS combined with a model for the solid-complex formation can successfully describe solid-liquid equilibria of glycol/methanol-water systems including the description of the solid-complex phase, which is known to exist at intermediate concentrations.

**General information**

State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Phase Equilibria and Separation Processes, Center for Energy Resources Engineering
Authors: Folas, G. (Intern), Gabrielsen, J. (Intern), Michelsen, M. L. (Intern), Stenby, E. H. (Intern), Kontogeorgis, G. (Intern)
Pages: 3823-3833
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- Web of Science (2018): Indexed yes
- BFI (2017): BFI-level 2
- Web of Science (2017): Indexed yes
- BFI (2016): BFI-level 2
- Scopus rating (2016): CiteScore 3.1 SJR 0.945 SNIP 1.139
- Web of Science (2016): Indexed yes
- BFI (2015): BFI-level 2
- Scopus rating (2015): SJR 0.949 SNIP 1.146 CiteScore 2.87
- Web of Science (2015): Indexed yes
- BFI (2014): BFI-level 2
- Scopus rating (2014): SJR 1.012 SNIP 1.292 CiteScore 2.85
- Web of Science (2014): Indexed yes
- BFI (2013): BFI-level 2
- Scopus rating (2013): SJR 0.982 SNIP 1.243 CiteScore 2.6
- ISI indexed (2013): ISI indexed yes
- Web of Science (2013): Indexed yes
- BFI (2012): BFI-level 2
- Scopus rating (2012): SJR 1.066 SNIP 1.338 CiteScore 2.56
- ISI indexed (2012): ISI indexed yes
- Web of Science (2012): Indexed yes
- BFI (2011): BFI-level 2
- Scopus rating (2011): SJR 1.086 SNIP 1.24 CiteScore 2.58
- ISI indexed (2011): ISI indexed yes
- Web of Science (2011): Indexed yes
- BFI (2010): BFI-level 2
- Scopus rating (2010): SJR 1.047 SNIP 1.165
- Web of Science (2010): Indexed yes
- BFI (2009): BFI-level 2
- Scopus rating (2009): SJR 1.002 SNIP 1.164
- Web of Science (2009): Indexed yes
- BFI (2008): BFI-level 2
- Scopus rating (2008): SJR 1.142 SNIP 1.267
- Web of Science (2008): Indexed yes
A field experiment was performed in a sandy vadose zone, studying the fate of an emplaced fuel-NAPL source, composed of 13 hydrocarbons and a tracer. The UNIFAC model was used to test the nonideal behavior of the source, and the numerical model MIN3P was used for assessing the effect of biodegradation on source evolution. The diffusive loss to the surrounding vadose zone and the atmosphere created temporary gradients in mole fractions of the individual compounds within the source NAPL. The evolution of the source composition corresponded in general with expectations based on Raoult’s Law, with the exception that the mole fractions of aromatic compounds in the source NAPL decreased faster than fractions of aliphatic compounds of similar volatility. Calculation of activity coefficients (gamma) using the UNIFAC model implied nonideal conditions, with composition-dependent gamma’s different from 1. Positive deviations were calculated for the aromatic compounds. The effect of biodegradation on source depletion, evaluated by numerical modeling, was greater for the aromatic as compared to the aliphatic compounds. Hence, the faster depletion of the aromatic relative to aliphatic compounds of similar volatility is both a result of the nonideality of the mixture and a result of partitioning and biodegradation in the pore-water. Vapor concentrations of the compounds in the source were in reasonable agreement with predictions based on the modified Raoult’s Law with the UNIFAC predicted gamma’s and the NAPL composition for the most volatile compounds. For the less volatile compounds, the measured vapor concentrations were lower than predicted with the largest deviations for the least volatile compounds. This field experiment illustrated that nonideal behavior and bioenhanced source depletion need to be considered at multicomponent NAPL spill sites.
Correlation and prediction of environmental properties of alcohol ethoxylate surfactants using the UNIFAC method

Environmental properties of one type of nonionic surfactants, the alcohol ethoxylates (polyoxyethylene alcohols), are predicted using the UNIFAC (universal quasi-chemical functional group activity coefficient) method. Various properties are considered: the octanol-water partition coefficient (Kow), the bioconcentration factor (BCF), and the toxicity. Kow values of alcohol ethoxylates are difficult to measure. Existing methods such as those in commercial software like ACD/ClogP and KowWin have not been applied to surfactants, and they fail for heavy alcohol ethoxylates (alkyl carbon numbers above 12). Thus, the Kow values are predicted here via UNIFAC and compared to the few available experimental data. Based on the predicted Kow values, a correlation between Kow and hydrophilic-lipophilic balance (HLB) is established because HLB is a widely used parameter in surfactant applications. Finally, BCF and toxicity of alcohol ethoxylates are correlated with their Kow. The proposed approach can be extended to other families of nonionic surfactants.

General information
State: Published
Organisations: Food Production Engineering, Department of Chemical and Biochemical Engineering, Center for Phase Equilibria and Separation Processes, Center for Energy Resources Engineering
Authors: Cheng, H. (Intern), Kontogeorgis, G. (Intern), Stenby, E. H. (Intern)
Pages: 7255-7261
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Main Research Area: Technical/natural sciences

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Journal: Industrial & Engineering Chemistry Research
Volume: 44
Issue number: 18
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BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.1 SJR 0.945 SNIP 1.139
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.949 SNIP 1.146 CiteScore 2.87
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.012 SNIP 1.292 CiteScore 2.85
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 0.982 SNIP 1.243 CiteScore 2.6
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.066 SNIP 1.338 CiteScore 2.56
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.086 SNIP 1.24 CiteScore 2.58
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.047 SNIP 1.165
Web of Science (2010): Indexed yes
We present solubility and diffusion data for the gases methane and carbon dioxide in the polymer poly(vinylidene fluoride). The polymer was cut from extruded piping intended for use in offshore oil and gas applications. Measurements were carried out using a purpose-built high-pressure microbalance. These properties were determined in the temperature range 80-120°C and in the pressure range 50-150 bar for methane and 20-40 bar for carbon dioxide. In general, good agreement was obtained for similar measurements reported in the literature. Solubility follows a Henry’s law (linear) dependence with pressure. Diffusion coefficients for each of the gases in the polymer were also measured using the balance. Activation energies for diffusion and heats of solution for the two gases in the polymer were also determined. © 2004 Elsevier Ltd. All rights reserved.
Experiments to determine the Solubility of methane and carbon dioxide in PA-11 have been performed in the temperature range 50-90°C and the pressure ranges 50-150 bar for methane and 20-40 bar for carbon dioxide. In general, the results agree fairly well with previous experiments for similar polymers, as well as showing correct trends in terms of temperature and pressure. The Solubility of the gases follows Henry's law-type behavior except for methane at very high pressures. Diffusivities were also measured for the same systems at the same conditions. While the diffusivities are subject to more uncertainty than the solubility measurements, the expected (Arrhenius) trends are observed. Agreement with other experimental data using different methods is also good.
Mathematical modeling of enzymatic hydrolysis of cellulosic model substrates

General information
State: Published
Organisations: Center for Microbial Biotechnology, Department of Systems Biology, Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering
Authors: Andersen, N. (Intern), Johansen, K. (Ekstern), Michelsen, M. (Ekstern), Stenby, E. H. (Intern), Olsson, L. (Intern)
Pages: S131-S132
Publication date: 2005
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Biotechnology
Volume: 118
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BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.88 SJR 0.978 SNIP 0.937
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.068 SNIP 0.987 CiteScore 2.87
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.113 SNIP 1.144 CiteScore 2.95
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.173 SNIP 1.188 CiteScore 3.22
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.255 SNIP 1.312 CiteScore 3.4
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.157 SNIP 1.064 CiteScore 2.87
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.126 SNIP 1.18
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.216 SNIP 1.235
Web of Science (2009): Indexed yes

Pressure parameters are added to the Extended UNIQUAC model presented by Thomsen and Rasmussen (1999). The improved model has been used for correlation and prediction of solid-liquid equilibrium (SLE) of scaling minerals (CaSO4, CaSO4·2H2O, BaSO4 and SrSO4) at temperatures up to 300°C and pressures up to 1000 bar. The results show that the Extended UNIQUAC model, with the proposed pressure parameters, is able to represent binary, ternary and quaternary solubility data within the experimental accuracy in the temperature range from -20 to 300°C, and the pressure range from 1 to 1000 bar.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Garcia, A. V. (Ekstern), Thomsen, K. (Intern), Stenby, E. H. (Intern)
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Journal: Geothermics
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BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.67 SJR 0.943 SNIP 1.417
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.344 SNIP 1.987 CiteScore 2.99
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Recent applications of the cubic-plus-association (CPA) equation of state to industrially important systems

The cubic-plus-association equation of state (CPA EoS) has been extended to phase equilibria of industrially important binary mixtures of alcohol-hydrocarbon, alcohol/glycol-water systems and mixtures with organic acids. The ability of the model to predict different types of equilibria was tested. Very satisfactory VLE and SLE prediction is achieved for alcohol-hydrocarbon systems, while the sensitivity of the LLE to the interaction parameter is demonstrated. It has been shown that CPA can perform VLE/LLE/SLE calculations in the case of alcohol-hydrocarbon binary systems with a single interaction parameter. Satisfactory SLE correlation of alcohol/glycol-water systems is achieved using a single interaction parameter over an extended temperature range. Moreover, satisfactory prediction was achieved for the multiphase equilibria of the mixture acetic acid-water-hexane based solely on binary interaction parameters. (c) 2004 Elsevier B.V. All rights reserved.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Phase Equilibria and Separation Processes, Center for Energy Resources Engineering
Authors: Folas, G. (Intern), Derawi, S. (Intern), Michelsen, M. L. (Intern), Stenby, E. H. (Intern), Kontogeorgis, G. (Intern)
Pages: 121-126
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Conference: 10th International Conference on Properties and Phase Equilibria for Product and Process Design, Snowbird, UT, United States, 16/05/2004 - 16/05/2004
Main Research Area: Technical/natural sciences

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Volume: 225
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BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 2.33 SJR 0.869 SNIP 1.155
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.874 SNIP 0.998 CiteScore 1.99
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 0.982 SNIP 1.248 CiteScore 2.28
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.007 SNIP 1.274 CiteScore 2.31
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.152 SNIP 1.286 CiteScore 2.31
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.034 SNIP 1.234 CiteScore 2.26
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 0.986 SNIP 1.317
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.133 SNIP 1.164
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.227 SNIP 1.09
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.031 SNIP 1.151
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.034 SNIP 1.245
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.009 SNIP 1.3
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 0.985 SNIP 1.349
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 1.193 SNIP 1.301
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 0.722 SNIP 1.101
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 0.966 SNIP 1.284
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 0.87 SNIP 0.898
Web of Science (2000): Indexed yes
Scopus rating (1999): SJR 0.938 SNIP 0.885

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DOIs:
Viscosity and Liquid Density of Asymmetric n-Alkane Mixtures: Measurement and Modelling

Viscosity and liquid density Measurements were performed, at atmospheric pressure, in pure and mixed n-decane, n-eicosane, n-docosane, and n-tetracosane from 293.15 K (or above the melting point) up to 343.15 K. The viscosity was determined with a rolling ball viscometer and liquid densities with a vibrating U-tube densimeter. Pure component results agreed, oil average, with literature values within 0.2% for liquid density and 3% for viscosity. The measured data were used to evaluate the performance of two models for their predictions: the friction theory coupled with the Peng-Robinson equation of state and a corresponding states model recently proposed for surface tension, viscosity, vapor pressure, and liquid densities of the series of n-alkanes. Advantages and shortcomings of these models are discussed.

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering
Authors: Queimada, A. J. (Ekstern), Marrucho, I. M. (Ekstern), Coutinho, J. A. (Ekstern), Stenby, E. H. (Intern)
Pages: 47-61
Publication date: 2005
Main Research Area: Technical/natural sciences

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Ratings:
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Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 0.332 SNIP 0.65 CiteScore 0.83
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.39 SNIP 0.979 CiteScore 0.9
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.466 SNIP 1.104 CiteScore 1.02
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.401 SNIP 1.311 CiteScore 1.13
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.371 SNIP 0.752 CiteScore 0.77
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.532 SNIP 1.112 CiteScore 1.08
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.455 SNIP 0.798
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.459 SNIP 0.849
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.563 SNIP 0.92
Wax Precipitation Modeled with Many Mixed Solid Phases

The behavior of the Coutinho UNIQUAC model for solid wax phases has been examined. The model can produce as many mixed solid phases as the number of waxy components. In binary mixtures, the solid rich in the lighter component contains little of the heavier component but the second phase shows substantial amounts of the lighter component dissolved in the heavier solid. Calculations have been performed taking into account the recrystallization of the solid alkanes into a second solid form. The Coutinho UNIQUAC model has been used to describe the lower-temperature solid phases. The higher-temperature mixed solid phase has been assumed to be either an ideal solution or to be described by Coutinho's Wilson activity coefficient model. This procedure accounts for more of the known behavior of mixed n-alkane solids. Comparison is also made with results assuming that all of the solid phases, both high-temperature and low-temperature forms, are pure. Model calculations compare well with the data of Pauly et al. for C18 to C30 waxes precipitating from n-decane solutions. (C) 2004 American Institute of Chemical Engineers.

General information
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Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Heidemann, R. A. (Ekstern), Madsen, J. (Ekstern), Stenby, E. H. (Intern), Andersen, S. I. (Intern)
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Journal: A I Ch E Journal
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Ratings:
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Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.11 SJR 1.034 SNIP 1.268
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Thermodynamic Modelling of Surfactant Solutions

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering
Direct measurement of gas solubilities in polymers with a high-pressure microbalance

Solubility and diffusion data are presented for methane and carbon dioxide gases in high-density polyethylene. The polymer was cut from extruded piping intended for use in offshore oil and gas applications. The measurements were carried out with a high-pressure microbalance. The properties were determined from 25 to 50°C and from 50 to 150 bar for methane and from 20 to 40 bar for carbon dioxide. In general, a good agreement was obtained with similar measurements reported in the literature. The solubility followed Henry's law (linear) dependence with pressure, except at high pressures for methane, for which negative deviations from Henry's law behavior were observed. The diffusion coefficients for each of the gases in the polymer were also measured with the balance, although the uncertainty was greater than for the solubility measurements. (C) 2003 Wiley Periodicals, Inc. J Appl Polym Sci 91: 1476-1488, 2004.
Application of the CPA equation of state to organic acids

The CPA (Cubic-Plus-Association) equation of state has been extended to modeling of organic acids. We will focus in this work on formic, acetic, and propanoic acids due to their importance to the chemical and petrochemical industries. Organic acids, unlike many other associating compounds, have a strong tendency to dimerise in the vapor phase at normal condition resulting in strong non-ideal behavior, even at low pressures. Pure compound parameters have been determined from vapor pressure and liquid density data for the three acids. Among the three tested association schemes (one-site, two-site, and four-site), only the one-site association scheme describes satisfactorily the association in both the gas and the liquid phase. Second virial coefficients are predicted well with the proposed one-site model. Excellent binary VLE and acceptable LLE correlations have been obtained for acid + aliphatic hydrocarbons employing a low value of a binary interaction parameter. (c) 2004 Elsevier B.V. All rights reserved.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Phase Equilibria and Separation Processes, Center for Energy Resources Engineering
Authors: Derawi, S. (Intern), Zeuthen, F. J. (Intern), Michelsen, M. L. (Intern), Stenby, E. H. (Intern), Kontogeorgis, G. (Intern)
Pages: 107-113
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Main Research Area: Technical/natural sciences

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BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 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
Characterisation of Oil-Gas Mixtures by Raman Spectroscopy

During oil- and gas exploration it is of importance to acquire information like composition and PVT properties at an early stage. At present analysis is done from considerable amounts of sample (litre scale) that need transportation to special laboratories. This procedure is very time consuming. The present project deals with development of a technique for quick analysis of oil-gas mixtures. The main emphasis is laid on characterisation of gas phases in equilibrium with oil at high pressures and high temperatures by Raman spectroscopy. The Raman technique has a great potential of being useful, due to its advantage of being, e.g. a non-destructive method. The spectra are obtained without touching the sample and only small amounts of sample are necessary (millilitres scale).

Detection of Occupancy Differences in Methane Gas Hydrates by Raman Spectroscopy

Gas hydrates are solid crystalline compounds, which grow from micro crystals to bulk masses resembling ordinary slush, snow or ice. Since gas hydrates exist at elevated pressures at temperatures well above the ice point, they can cause severe problems under production and transportation of reservoir fluids due to plugging. Methods to prevent hydrate formation are in use, e.g. by injection of inhibitors. From environmental and security points of view an easy way to detect
hydrate formation is of interest. We have tried to detect methane hydrate formation by use of Raman spectroscopy.
Extension of the CPA equation of state to organic acids

General information

State: Published
Organisations: Department of Chemical and Biochemical Engineering
Authors: Kontogeorgis, G. (Intern), Derawi, S. (Intern), Zeuthen, F. J. (Intern), Michelsen, M. L. (Intern), Stenby, E. H. (Intern)
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.
Streamline Simulation with Capillary Effects Applied to Petroleum Engineering Problems

**General information**

- **State:** Published
- **Organisations:** Department of Chemical and Biochemical Engineering, Center for Phase Equilibria and Separation
- **Authors:** Berenblyum, R. (Intern), Stenby, E. H. (Intern), Michelsen, M. L. (Intern), Shapiro, A. (Intern)
- **Publication date:** 2004

**Publication information**

- **Original language:** English
- **Main Research Area:** Technical/natural sciences
- **Roman A Berenblyum, ph.d..pdf**
- **Source:** orbit
- **Source-ID:** 209193
- **Publication:** Research - peer-review › Journal article – Annual report year: 2004

**Theoretical and experimental comparison of the Soret coefficient for water-methanol and water-ethanol binary mixtures**

In multicomponent mixtures, a much richer variety of phenomena can occur than in simple (single-component) fluids. Natural convection in single-component fluids is due to buoyancy forces caused by temperature gradients. In multicomponent mixtures, buoyancy forces may also be caused by concentration gradients. Because natural convection, molecular diffusion, and thermal conduction have different relaxation time scales, a wide variety of resulting convective motions and heat, and mass distributions might occur. In some fluid mixtures such as water-ethanol system, for instance, ethanol diffuses much more slowly than heat, and because of this difference in time scales oscillatory convection might occur. In a multicomponent mixture, the total molar flux consists of two parts: the convective molar flux and the diffusive molar flux (resulting from the difference between the component, velocity and the bulk velocity). The diffusion molar flux of a component depends, not only, on its own mole fraction gradient (Fickian diffusion), but also on the gradient of all the components present in the mixture (cross-molecular diffusion). The diffusion flux depends also on the pressure gradient (pressure diffusion; the so-called gravitational effect) and temperature gradient (thermal diffusion; the so-called Soret effect). Firoozabadi’s thermal diffusion model was applied to calculate the Soret coefficient, as well as the thermal diffusion...
coefficient and molecular diffusion coefficient for methanol-water and ethanol-water mixtures at 310.6.5 K temperature and 1 bar pressure with 10% water mass fraction. The results were compared with experimental data (J.K. Platten. in Proceedings of the 5th, International Meeting on Thermodiffusion, (IMT5); Lyngby Aug, 2002 Philos. Mag. 83. Nos. 17-18 (2003)), as well as theoretical predictions with other models. A better agreement with the experimental data using the Firoozabadi model was achieved.

**General information**

State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Phase Equilibria and Separation Processes, Center for Energy Resources Engineering, Ryerson University, University of Toronto
Authors: Saghir, M. (Ekstern), Jiang, C. (Ekstern), Derawi, S. (Intern), Stenby, E. H. (Intern), Kawaji, M. (Ekstern)
Pages: 241-247
Publication date: 2004
Conference: International Meeting on Thermal Forces, Varenna, ITALY, 01/01/2004
Main Research Area: Technical/natural sciences

**Publication information**

Volume: 15
Issue number: 3
ISSN (Print): 1292-8941
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 2
Scopus rating (2016): SJR 0.412 SNIP 0.537 CiteScore 0.95
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.583 SNIP 0.659 CiteScore 1.1
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 0.565 SNIP 0.569 CiteScore 1.05
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 0.694 SNIP 0.937 CiteScore 1.5
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 0.853 SNIP 0.795 CiteScore 1.5
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 0.866 SNIP 0.924 CiteScore 1.49
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.068 SNIP 0.928
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 0.963 SNIP 0.884
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 0.99 SNIP 0.859
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.279 SNIP 1.019
Scopus rating (2006): SJR 1.419 SNIP 1.041
Scopus rating (2005): SJR 1.509 SNIP 1.093
Scopus rating (2004): SJR 1.399 SNIP 1.067
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 1.274 SNIP 1.088
Scopus rating (2002): SJR 1.04 SNIP 1.325
Web of Science (2002): Indexed yes
Three-phase Compositional Streamline Simulation and Its Application to WAG

**General information**
- **State:** Published
- **Organisations:** Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
- **Authors:** Yan, W. (Intern), Michelsen, M. L. (Intern), Stenby, E. H. (Intern), Berenblyum, R. (Intern), Shapiro, A. (Intern)
- **Number of pages:** 11
- **Publication date:** 2004
- **Event:** Paper presented at SPE/DOE Symposium on Improved Oil Recovery, Tulsa, Oklahoma.
- **Main Research Area:** Technical/natural sciences
- **DOIs:** 10.1140/epje/i2004-10063-7

Upgrade of an old Raman Spectrometer

Improvement of a conventional Jeol Raman spectrometer with a single channel photo multiplier detector is described. New optical components (fibres, mirror, lens and CCD detector) have been chosen to design a high quality and easy-to-use instrument. Tests have shown that with this modified spectrometer Raman spectra can be acquired of a quality comparable to the spectra obtained previously, but the time needed to obtain a spectrum is markedly reduced. Selected test spectra and a simple calibration procedure to obtain the wavenumber values from the band CCD pixel position are presented.

**General information**
- **State:** Published
- **Organisations:** Department of Chemistry, Department of Chemical and Biochemical Engineering
- **Authors:** Hansen, S. B. (Intern), Berg, R. W. (Intern), Stenby, E. H. (Intern)
- **Pages:** 385-397
- **Publication date:** 2004
- **Main Research Area:** Technical/natural sciences

**Publication information**
- **Journal:** Applied Spectroscopy Reviews
- **Volume:** 39
- **Issue number:** 3
- **ISSN (Print):** 0570-4928
- **Ratings:**
  - BFI (2018): BFI-level 1
  - Web of Science (2018): Indexed yes
  - BFI (2017): BFI-level 1
  - Web of Science (2017): Indexed Yes
  - BFI (2016): BFI-level 1
  - Scopus rating (2016): CiteScore 4.82 SJR 0.937 SNIP 2.199
  - BFI (2015): BFI-level 1
  - Scopus rating (2015): SJR 0.928 SNIP 1.892 CiteScore 4.27
  - Web of Science (2015): Indexed yes
  - BFI (2014): BFI-level 1
  - Scopus rating (2014): SJR 1.199 SNIP 1.947 CiteScore 4.36
Upgrade of a Raman Spectrometer

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Hansen, S. B. (Ekstern), Berg, R. W. (Ekstern), Stenby, E. H. (Intern)
Pages: 385-397
Publication date: 2004
Main Research Area: Technical/natural sciences

Publication information
Journal: Applied Spectroscopy Reviews
Volume: 39
Issue number: 3
ISSN (Print): 0570-4928
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
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
A Corresponding States Model for the Estimation of Thermophysical Properties of Asymmetric Mixtures

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Queimada, A. J. (Ekstern), Marrucho, I. M. (Ekstern), Stenby, E. H. (Intern), Coutinho, J. A. (Ekstern)
Publication date: 2003
Event:
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 41110
Publication: Research › Poster – Annual report year: 2003

A new Corresponding States model for the estimation of thermophysical properties of long chain n-alkanes

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Queimada, A. J. (Ekstern), Stenby, E. H. (Intern), Marrucho, I. M. (Ekstern), Coutinho, J. A. (Ekstern)
Pages: 303-314
Publication date: 2003
Main Research Area: Technical/natural sciences

Publication information
Journal: Fluid Phase Equilibria
Volume: 212
Issue number: 1
ISSN (Print): 0378-3812
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 2.33 SJR 0.869 SNIP 1.155
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.874 SNIP 0.998 CiteScore 1.99
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 0.982 SNIP 1.248 CiteScore 2.28
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.007 SNIP 1.274 CiteScore 2.31
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.152 SNIP 1.286 CiteScore 2.31
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.034 SNIP 1.234 CiteScore 2.26
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
The Cubic Plus Association (CPA) equation of state is a thermodynamic model, which combines the well-known cubic SRK (Soave-Redlich-Kwong) equation of state and the association term proposed by Wertheim, typically employed in models like SAFT (statistical associating fluid theory). CPA has been shown in the past to be a successful model for phase equilibria calculations for systems containing water, hydrocarbons and alcohols. In this work, CPA is applied for the first time to liquid-liquid equilibria (LLE) for systems containing glycols and hydrocarbons. It is shown that excellent correlation is achieved with solely a single interaction parameter per binary system. The correlation procedure as well as the nature of the experimental data play a crucial role in the parameter estimation and they are thus extensively discussed. (C) 2003 Elsevier Science B.V. All rights reserved.
Application of the CPA equation of state to industrially important systems

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Derawi, S. (Intern), Michelsen, M. L. (Intern), Kontogeorgis, G. (Intern), Stenby, E. H. (Intern)
Publication date: 2003
Event: Poster session presented at 15 Years of the SAFT Equation, Barcelona, Spain.
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 41363
Publication: Research › Poster – 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
Authors: Derawi, S. (Intern), Michelsen, M. L. (Intern), Kontogeorgis, G. (Intern), Stenby, E. H. (Intern)
Publication date: 2003
Event: Abstract from 20th European Symposium on Applied Thermodynamics, Lahnstein, Germany.
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 41353
Publication: Research › Conference abstract for conference – Annual report year: 2003

Application of the CPA Equation of State to Industrially Important Systems

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Derawi, S. O. (Ekstern), Michelsen, M. L. (Intern), Kontogeorgis, G. (Intern), Stenby, E. H. (Intern)
Publication date: 2003
Event: Poster session presented at 20th European Symposium on Applied Thermodynamics, Lahnstein, Germany.
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 209197
Publication: Research › Poster – Annual report year: 2003

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
Authors: Derawi, S. (Intern), Folas, G. (Ekstern), 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 Ressources Engineering, Department of Chemical and Biochemical Engineering, Center for Biological Sequence Analysis, Department of Systems Biology, Center for Energy Resources
Black Oil Streamline Simulator with Capillary Effects

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Berenblyum, R. (Ekstern), Shapiro, A. (Intern), Jessen, K. (Ekstern), Stenby, E. H. (Intern), Orr Jr., F. M. (Ekstern)
Publication date: 2003
Event:
Main Research Area: Technical/natural sciences

Bibliographical note
pub.interno: SEP0316
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WWWWW: cataloguer/id is not the CWIS of the main author
Source: orbit
Source-ID: 41367
Publication: Research › Poster – 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 Ressources Engineering
Authors: Berenblyum, R. (Intern), Shapiro, A. (Intern), Jessen, K. (Intern), Stenby, E. H. (Intern), Orr Jr., F. (Ekstern)
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

Compositional Streamline Simulation: Progress Report No. 4

General information
State: Published
Organisations: CERE – Center for Energy Ressources Engineering, Department of Chemical and Biochemical Engineering
Authors: Yan, W. (Intern), Berenblyum, R. (Intern), Shapiro, A. (Intern), Michelsen, M. L. (Intern), Stenby, E. H. (Intern)
Publication date: 2003

Publication information
Original language: English
Detection of Dew-Point by substantial Raman Band Frequency Jumps (A new Method)

General information
State: Published
Organisations: Department of Chemistry, Department of Chemical and Biochemical Engineering
Authors: Hansen, S. B. (Intern), Berg, R. W. (Intern), Stenby, E. H. (Intern)
Publication date: 2003
Main Research Area: Technical/natural sciences
Links:
Source: orbit
Source-ID: 39189
Publication: Research - peer-review › Poster – Annual report year: 2003

Evaluation of the Thermodynamic Models for the Thermal Diffusion Factor

Over the years, several thermodynamic models for the thermal diffusion factors for binary mixtures have been proposed. The goal of this paper is to test some of these models in combination with different equations of state. We tested the following models: those proposed by Rutherford and Drickamer in 1954, by Dougherty and Drickamer in 1955, by Haase in 1969, by Kempers in 1989 and 2002, and by Shucla and Firoozabadi in 1998. The calculated values of thermal diffusion factors were compared with a few sets of experimental data for hydrocarbon mixtures. For calculation of the partial molar properties we applied different thermodynamic models, such as the Soave-Redlich-Kwong and the Peng-Robinson equations of state. The necessity to try different thermo-dynamic models is caused by the high sensitivity of the thermal diffusion factors to the values of the partial molar properties. Two different corrections for the determination of the partial molar volumes have been implemented; the Peneloux correction and the correction based on the principle of corresponding states.

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Gonzalez-Bagnoli, M. G. (Ekstern), Shapiro, A. (Intern), Stenby, E. H. (Intern)
Pages: 2171-2183
Publication date: 2003
Main Research Area: Technical/natural sciences

Publication information
Volume: 83
ISSN (Print): 1478-6435
Ratings:
BFI (2018): BFI-level 1
Extension of the CPA Equation of State to Glycol-Water Cross-Associating Systems

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering
Authors: Derawi, S. (Intern), Kontogeorgis, G. (Intern), Michelsen, M. L. (Intern), Stenby, E. H. (Intern)
Pages: 1470-1477
Publication date: 2003
Extension of the cubic-plus-association equation of state to glycol-water cross-associating systems

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Derawi, S. (Intern), Michelsen, M. L. (Intern), Kontogeorgis, G. (Intern), Stenby, E. H. (Intern)
Pages: 1470-1477
Publication date: 2003
Main Research Area: Technical/natural sciences

Publication information
Journal: Industrial & Engineering Chemistry Research
Volume: 42
Issue number: 7
ISSN (Print): 0888-5885
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.1 SJR 0.945 SNIP 1.139
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.949 SNIP 1.146 CiteScore 2.87
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.012 SNIP 1.292 CiteScore 2.85
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 0.982 SNIP 1.243 CiteScore 2.6
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.066 SNIP 1.338 CiteScore 2.56
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.086 SNIP 1.24 CiteScore 2.58
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.047 SNIP 1.165
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.002 SNIP 1.164
Web of Science (2009): Indexed yes
Friction Theory Prediction of Crude Oil Viscosity at Reservoir Conditions Based on Dead Oil Properties

The general one-parameter friction theory (f-theory) models have been further extended to the prediction of the viscosity of real "live" reservoir fluids based on viscosity measurements of the "dead" oil and the compositional information of the live fluid. This work representation of the viscosity of real fluids is obtained by a simple one-parameter tuning of a linear equation derived from a general one-parameter f-theory model. Further, this is achieved using simple cubic equations of state (EOS), such as the Peng-Robinson (PR) EOS or the Soave-Redlich-Kwong (SRK) EOS, which are commonly used within the oil industry. In sake of completeness, this work also presents a simple characterization procedure which is based on compositional information of an oil sample. This procedure provides a method for characterizing an oil into a number of compound groups along with the critical constants and parameters that are required by an EOS. The resulting EOS characterized fluid correctly reproduces properties such as the saturation pressure and the liquid phase density, from reservoir conditions to low pressure conditions. The viscosity modeling approach along with the characterization method presented in this work provide a complete self-consistent procedure for the viscosity and density modeling of reservoir fluids. (C) 2003 Elsevier B.V. All rights reserved.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Phase Equilibria and Separation Processes, Center for Energy Resources Engineering
Authors: Cisneros, S. (Intern), Zeberg-Mikkelsen, C. K. (Intern), Stenby, E. H. (Intern)
Pages: 233-243
Publication date: 2003
Main Research Area: Technical/natural sciences

Publication information
Journal: Fluid Phase Equilibria
Volume: 212
Issue number: 1-2
ISSN (Print): 0378-3812
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Original language: English

classification, equation of state, f-theory, modeling, petroleum, viscosity

DOIs:
10.1016/S0378-3812(03)00263-2

Source: orbit
Source-ID: 41227
Generalized Relation Between Surface Tension and Viscosity: a Study on Pure and Mixed n-Alkanes

**General information**
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Queimada, A. J. (Ekstern), Marrucho, I. M. (Ekstern), Stenby, E. H. (Intern), Coutinho, J. A. (Ekstern)
Publication date: 2003

**Host publication information**
Title of host publication: 15th Symposium on Thermophysical Properties, Boulder, Colorado
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 41113
Publication date: 2003

Measurement and Modelling of Gas Solubility and Diffusivity in Polymers at High Pressure and Temperature

**General information**
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering
Authors: von Solms, N. (Intern), Rubin, A. (Ekstern), Andersen, S. I. (Intern), Stenby, E. H. (Intern)
Publication date: 2003

**Host publication information**
Title of host publication: Proceedings of the AIChE Annual Meeting 2003
Publisher: American Institute of Chemical Engineers
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 41316
Publication date: 2003

Modeling of the water-hydrocarbon interface: Coupling the CPA EoS with the gradient theory

**General information**
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Queimada, A. J. (Ekstern), Marrucho, I. M. (Ekstern), Stenby, E. H. (Intern), Kontogeorgis, G. (Intern), Miqueu, C. (Ekstern), Coutinho, J. A. (Ekstern)
Pages: 391-394
Publication date: 2003

**Host publication information**
Title of host publication: ESAT 2003, Germany
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 41365
Publication date: 2003

Supercritical Fluid Extraction of a-Methylene-g-Butyrolactone from Alstroemeria: Optimization by Statistical Experimental Design

**General information**
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Hutchenson, K. W. (Ekstern), Jensen, O. F. (Ekstern), Kao, C. P. (Ekstern), Stenby, E. H. (Intern)
Publication date: 2003
Termodynamiske modeler for produktionskemikaliers egenskaber

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering
Authors: Derawi, S. (Intern), Michelsen, M. L. (Intern), Kontogeorgis, G. (Intern), Stenby, E. H. (Intern)
Pages: 15-17
Publication date: 2003
Main Research Area: Technical/natural sciences

Publication information
Journal: Dansk Kemi
Volume: 84
ISSN (Print): 0011-6335
Ratings:
ISI indexed (2013): ISI indexed no
ISI indexed (2012): ISI indexed no
ISI indexed (2011): ISI indexed no
Web of Science (2007): Indexed yes
Web of Science (2004): Indexed yes
Original language: Danish
Source: orbit
Source-ID: 138316
Publication: Communication › Journal article – Annual report year: 2003

Upgrade of an Raman Spectrometer

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering
Authors: Hansen, S. B. (Intern), Berg, R. (Ekstern), Stenby, E. H. (Intern)
Pages: 20
Publication date: 2003
Main Research Area: Technical/natural sciences

Publication information
Journal: Applied Spectroscopy
Volume: 0
Issue number: 0
ISSN (Print): 0003-7028
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 0.48 SNIP 0.967 CiteScore 1.76
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.649 SNIP 1.09 CiteScore 1.96
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Viscosity and Density Modeling and Prediction of Reservoir Fluids: from Natural Gas to Heavy Oils

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Quiñones-Cisneros, S. E. (Ekstern), Zéberg-Mikkelsen, C. K. (Ekstern), Baylaucq, A. (Ekstern), Boned, C. (Ekstern), Stenby, E. H. (Intern)
Pages: 395-398
Publication date: 2003

Host publication information
Title of host publication: ESAT 2003
Main Research Area: Technical/natural sciences
Viscosity and Liquid Density of Asymmetric Hydrocarbon Mixtures

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Queimada, A. J. (Ekstern), Cisneros, S. (Intern), Marrucho, I. M. (Ekstern), Coutinho, J. A. (Ekstern), Stenby, E. H. (Intern)
Pages: 1221-1240
Publication date: 2003
Main Research Area: Technical/natural sciences

Publication information
Journal: International Journal of Thermophysics
Volume: 24
Issue number: 5
ISSN (Print): 0195-928X
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 0.332 SNIP 0.65 CiteScore 0.83
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.39 SNIP 0.979 CiteScore 0.9
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.466 SNIP 1.104 CiteScore 1.02
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.401 SNIP 1.311 CiteScore 1.13
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.371 SNIP 0.752 CiteScore 0.77
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.532 SNIP 1.112 CiteScore 1.08
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.455 SNIP 0.798
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.459 SNIP 0.849
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.563 SNIP 0.92
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 0.599 SNIP 0.915
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 0.729 SNIP 1.002
Scopus rating (2005): SJR 0.754 SNIP 1.267
Web of Science (2005): Indexed yes
Viscosity Modeling and Prediction of Reservoir Fluids: from Natural Gas to Heavy Oils

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Cisneros, S. (Intern), Zeberg-Mikkelsen, C. K. (Intern), Baylaucq, A. (Ekstern), Boned, C. (Ekstern), Stenby, E. H. (Intern)
Publication date: 2003

Host publication information
Title of host publication: 15th Symposium on Thermophysical Properties, Boulder, Colorado
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 41097
Publication: Research › Conference abstract in proceedings – Annual report year: 2003

Accurate Density and Viscosity Modeling of Non-Polar Fluids Based on the f-theory

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Cisneros, S. (Intern), Zeberg-Mikkelsen, C. K. (Intern), Stenby, E. H. (Intern)
Pages: 41-55
Publication date: 2002
Main Research Area: Technical/natural sciences

Publication information
Journal: International Journal of Thermophysics
Volume: 23
Issue number: 1
ISSN (Print): 0195-928X
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 0.332 SNIP 0.65 CiteScore 0.83
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.39 SNIP 0.979 CiteScore 0.9
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.466 SNIP 1.104 CiteScore 1.02
Characterization of Oil-Gas Mixtures by Raman Spectroscopy

General information
State: Published
Organisations: Department of Chemistry, Energy and Materials, Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering
Authors: Hansen, S. B. (Intern), Berg, R. W. (Intern), Stenby, E. H. (Intern)
Publication date: 2002
Event: Abstract from Annual Discussion Meeting of IVC-SEP, Marienlyst, Elsinore, Denmark, .
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 40972
Publication: Research › peer-review › Journal article – Annual report year: 2002

Detection of Occupancy Differences in Methane Gas Hydrates by Raman Spectroscopy

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Department of Chemistry, Center for Energy Resources Engineering
Detection of Occupancy Differences in Methane Gas Hydrates by Raman Spectroscopy.

Effect of Geothermal Gradients on Fluid Distribution in Petroleum Reservoirs

General one-parameter friction theory viscosity model for the Patel-Teja EOS

How to determine the pressure of a methane-containing gas mixture by means of two weak Raman bands, v(3) and 2v(2)
function of pressure. Surprisingly it is observed that the ratio at a fixed pressure is independent of the composition and thereby of the surroundings in which the methane molecule is vibrating. A model function to predict the pressure is given. From a practical point of view, the present results could be useful for determining directly the total pressure in methane mixtures the composition of which is not known.

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Department of Chemistry, Center for Energy Resources Engineering
Authors: Hansen, S. B. (Intern), Berg, R. W. (Intern), Stenby, E. H. (Intern)
Pages: 160-164
Publication date: 2002
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Raman Spectroscopy
Volume: 33
Issue number: 3
Original language: English
Source: orbit
Source-ID: 40878
Publication: Research - peer-review › Journal article – Annual report year: 2002

Interplay of Phase Behavior and Numerical Dispersion in Finite Difference Compositional Simulation

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Phase Equilibria and Separation Processes, Center for Energy Resources Engineering
Authors: Jessen, K. (Intern), Stenby, E. H. (Intern), Orr Jr., F. (Ekstern)
Pages: 1-15
Publication date: 2002
Main Research Area: Technical/natural sciences

Publication information
Journal: S P E Journal
Volume: 0
ISSN (Print): 1086-055X
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 0.95 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
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, methylcyclohexane (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.
Modeling of Phase Equilibria Containing Associating Fluids

In recent years, there has been an increasing interest of the petrochemical industry in modeling of the partitioning of production chemicals e.g. gas hydrate inhibitors, corrosion inhibitors, solvents etc. between the crude oil and water. This requires basically a thermodynamic model either in terms of an activity coefficient model or an equation of state. Our
target in this thesis is to review and develop such models capable of describing qualitatively as well as quantitatively phase equilibria in multicomponent multiphase systems containing non-polar, polar, and associating compounds. The background and main targets for this thesis are presented in Chapter 1. In Chapter 2, a comprehensive review of the application of group contribution (GC) models such as various forms of UNIFAC and the so-called AFC (Atom and Fragment Contributions) correlation model for Pow (octanol-water partition coefficient) calculations has been carried out. UNIFAC is an activity coefficient model while AFC is a model specifically developed for Pow calculations. Five different versions of UNIFAC and the AFC correlation model have been compared with each other and with experimental data. The range of applicability of the GC models to Pow is discussed, and general conclusions are obtained. A thorough analysis of the models was conducted including residual plots and numerical and graphical comparisons. We conclude that the group-contribution concept has possibly exhausted its applicability to account for highly asymmetric systems, especially for aqueous solutions with complex poly-functional chemicals. In Chapter 3, liquid-liquid equilibrium data for 7 binary glycol-hydrocarbon systems have been measured in the temperature range 32 °C to 80 °C and pressure equal to 1 bar. The measured systems are monoethylene glycol + heptane, methylcyclohexane, hexane, propylene glycol + heptane, diethylene glycol + heptane, triethylene glycol + heptane, and tetraethylene glycol + 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 two temperature dependent models with an average deviation in the composition for both phases of 3 % for both NRTL and UQ 4 while deviation is 15 % for UQ 2. These results indicate the necessity of using the linearly dependent interaction parameters. The CPA equation of state is a thermodynamic model, which combines the well-known cubic SRK equation of state and the association term proposed by Wertheim, typically employed in models like the various variations of SAFT. CPA has been shown in the past to be a successful model for phase equilibria calculations for systems containing water, hydrocarbons and alcohols. In Chapter 4, CPA is applied for the first time to liquid-liquid equilibria for systems containing glycols and hydrocarbons. It is shown that excellent correlation is achieved with solely a single interaction parameter per binary system. The correlation procedure as well as the nature of the experimental data play a crucial role in the parameter estimation and they are thus extensively discussed. In Chapter 5, the application of the CPA equation of state is extended to mixtures containing cross-associating compounds such as glycols and water. In this case, combining rules are required in the association term of CPA for the cross-association energy and volume parameters. Different types of such combining rules have been suggested over the past years for association models such as SAFT. These are tested in this work for CPA in terms of their correlation and prediction capabilities for vapor-liquid equilibria of glycol-water systems. Comparisons with SRK are also provided. It was found, that the arithmetic mean combining rule for the cross-association energy parameter and the geometric mean for the cross-association volume parameter provide overall the best results for cross-associating systems containing glycols and water. Moreover, preliminary results show that the CPA model can be used to predict multi-component, multiphase equilibria for glycol/water/hydrocarbon mixtures based solely on binary interaction parameters. In Chapter 6, conclusions and suggestions for future work are presented.

Modelling the Acid Restimulation of Carbonate Fractured Injection Wells in a North Sea

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Phase Equilibria and Separation Processes, Center for Energy Resources Engineering
Authors: Berenblyum, R. (Intern), Hansen, J. H. (Ekstern), Michelsen, M. L. (Intern), Shapiro, A. (Intern), Stenby, E. H. (Intern)
Publication date: 2002
Multicomponent Adsorption: Principles and Models

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering
Authors: Shapiro, A. (Intern), Stenby, E. H. (Intern)
Number of pages: 878
Publication date: 2002

Host publication information
Title of host publication: Adsorption: Theory, Modeling, and Analysis
Publisher: C R C Press LLC
Editor: Tóth, J.
Edition: 1
ISBN (Print): 0824707478

Series: Surfactant Science Series
Number: 107
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 250821
Publication: Research - peer-review › Book chapter – Annual report year: 2001

Nanotechnology at KT

General information
State: Published
Organisations: CHEC Research Centre, Department of Chemical and Biochemical Engineering, The Danish Polymer Centre, Membrane Technology group, Center for Phase Equilibria and Separation Processes, Computer Aided Process Engineering Center
Authors: Glarborg, P. (Intern), Hassager, O. (Intern), Jonsson, G. E. (Intern), Stenby, E. H. (Intern), Gani, R. (Intern)
Publication date: 2002

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 40847
Publication: Research › Report – Annual report year: 2002

Prediction of micelle formation for aqueous polyoxyethylene alcohol solutions with the UNIFAC model

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Cheng, H. (Intern), Kontogeorgis, G. (Intern), Stenby, E. H. (Intern)
Pages: 892-898
Publication date: 2002
Main Research Area: Technical/natural sciences

Publication information
Journal: Industrial & Engineering Chemistry Research
Volume: 41
Issue number: 5
ISSN (Print): 0888-5885
Ratings:
BFI (2018): BFI-level 2
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Original language: English
Source: orbit
Source-ID: 40871
Publication: Research - peer-review › Journal article – Annual report year: 2002
Prediction of Octanol-Water Partition Coefficients of Surfactants with Engineering Methods

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Cheng, H. (Intern), Kontogeorgis, G. (Intern), Stenby, E. H. (Intern)
Publication date: 2002

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 40948
Publication: Research - peer-review › Report – Annual report year: 2002

Principle of Entropy Maximization for Nonequilibrium Steady States
The goal of this contribution is to find out to what extent the principle of entropy maximization, which serves as a basis for the equilibrium thermodynamics, may be generalized onto non-equilibrium steady states. We prove a theorem that, in the system of thermodynamic coordinates, where entropy has a maximum in a steady state with regard to some thermodynamic variables, the matrix of the Onsager phenomenological coefficients becomes diagonal. The theorem requires consistent rules of the coordinate transformations in the non-equilibrium thermodynamics. Such rules are formulated. The results make it possible, in some cases, to reduce the number of unknown transport coefficients in thermodynamic description of the transport processes.

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Shapiro, A. (Intern), Stenby, E. H. (Intern)
Pages: 61-73
Publication date: 2002
Main Research Area: Technical/natural sciences

Publication information
Journal: Lecture Notes in Physics
Volume: 584
ISSN (Print): 1616-6361
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 0.591 SNIP 0.382 CiteScore 0.55
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.661 SNIP 0.428 CiteScore 0.8
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.815 SNIP 0.509 CiteScore 1.12
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.542 SNIP 0.426 CiteScore 0.75
ISI indexed (2013): ISI indexed no
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.363 SNIP 0.36 CiteScore 0.48
ISI indexed (2012): ISI indexed no
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.396 SNIP 0.288 CiteScore 0.53
ISI indexed (2011): ISI indexed no
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.44 SNIP 0.339
BFI (2009): BFI-level 1
Raman Spectroscopic investigations of gas mixtures.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Department of Chemistry
Authors: Hansen, S. B. (Intern), Berg, R. W. (Intern), Stenby, E. H. (Intern)
Pages: 15-18
Publication date: 2002
Main Research Area: Technical/natural sciences

Publication information
Journal: Dansk Kemi
Volume: 83
Issue number: 12
ISSN (Print): 0011-6335
Ratings:
ISI indexed (2013): ISI indexed no
ISI indexed (2012): ISI indexed no
ISI indexed (2011): ISI indexed no
Web of Science (2007): Indexed yes
Web of Science (2004): Indexed yes
Original language: English
Source: orbit
Source-ID: 42893
Publication: Communication › Journal article – Annual report year: 2002

Research at KT 2002

General information
State: Published
Organisations: CHEC Research Centre, Department of Chemical and Biochemical Engineering, The Danish Polymer Centre, Computer Aided Process Engineering Center, CERE – Center for Energy Resources Engineering
Authors: Glarborg, P. (Intern), Hassager, O. (Intern), Jonsson, G. E. (Intern), Stenby, E. H. (Intern), Gani, R. (Intern)
Publication date: 2002

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 40843
Publication: Research › Report – Annual report year: 2002

Scale Formation in Geothermal Plants

General information
State: Published
Simulation of Gas Injection Processes

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Phase Equilibria and Separation Processes
Authors: Jákupsstovu, S. I. (Intern), Stenby, E. H. (Intern)
Publication date: 2002

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Electronic versions:
sigurd jakup, ph.d.pdf
Source: orbit
Source-ID: 192210
Publication: Research › Ph.D. thesis – Annual report year: 2002

Viscosity modeling and prediction of crude oils

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Cisneros, S. (Intern), Stenby, E. H. (Intern)
Publication date: 2002

Event:
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 40954
Publication: Research › Conference abstract for conference – Annual report year: 2002

Viscosity modeling of associating fluids based on the friction theory: pure alcohols

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Zeberg-Mikkelsen, C. K. (Intern), Cisneros, S. (Intern), Stenby, E. H. (Intern)
Pages: 1191-1203
Publication date: 2002

Main Research Area: Technical/natural sciences

Publication information
Journal: Fluid Phase Equilibria
Volume: 194
Issue number: 0
ISSN (Print): 0378-3812
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Viscosity prediction of carbon dioxide plus hydrocarbon mixtures using the friction theory

The general one-parameter f-theory model has been used in conjunction with the SRK and the PR EOS to predict the viscosity of well-defined carbon dioxide + hydrocarbon mixtures. The predicted viscosities are within the uncertainty appropriate for most industrial applications. Although the studied mixtures are simple representations or real oil mixtures with carbon dioxide, the f-theory approach can easily be extended to more complex scenarios, such as the simulation of carbon dioxide enhance oil recovery. Additionally, a comparison with the LBC model, which is a widely used model in the oil industry, has been carried Out. In contrast to the f-theory models, the strong dependency that the LBC model has on the accuracy or the density is clearly evident for the kind Of Mixtures Studied in this work. Furthermore, it is shown how the phase behavior complexity that carbon dioxide + hydrocarbon mixtures develop may have a direct influence on the performance of the viscosity modeling and prediction.
Viscosity Prediction of Natural Gas Using the Friction Theory

Based on the concepts of the friction theory (f-theory) for viscosity modeling, a procedure is introduced for predicting the viscosity of hydrocarbon mixtures rich in one component, which is the case for natural gases. In this procedure, the mixture friction coefficients are estimated with mixing rules based on the values of the pure component friction coefficients. Since natural gases contain mainly methane, two f-theory models are combined, where the friction coefficients of methane are estimated by a seven-constant f-theory model directly fitted to methane viscosities, and the friction coefficients of the other components are estimated by the one-parameter general f-theory model. The viscosity predictions are performed with the SRK, the PR, and the PRSV equations of state, respectively. For recently measured viscosities of natural gases, the resultant AAD (0.5 to 0.8%) is in excellent agreement with the experimental uncertainty (+/-1.0%). The AAD is found to be higher for older measurements (around 3.5%), due mainly to the higher experimental uncertainties and problems with some of the measurements. Overall, the results are satisfactory for most industrial applications related to natural gases.

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Zeberg-Mikkelsen, C. K. (Intern), Cisneros, S. (Intern), Stenby, E. H. (Intern)
Pages: 437-454
Publication date: 2002
Main Research Area: Technical/natural sciences

Publication information
Journal: International Journal of Thermophysics
Volume: 23
Issue number: 2
ISSN (Print): 0195-928X
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 0.332 SNIP 0.65 CiteScore 0.83
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.39 SNIP 0.979 CiteScore 0.9
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.466 SNIP 1.104 CiteScore 1.02
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.401 SNIP 1.311 CiteScore 1.13
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.371 SNIP 0.752 CiteScore 0.77
**Determination of Relative Permeability - Analysis of Experimental Methods**

**General information**
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering
Authors: Poulsen, S. (Intern), Stenby, E. H. (Intern)
Publication date: Sep 2001

**Publication information**
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 209353
Publication: Research - peer-review › Journal article – Annual report year: 2002

**Viscosity Study of Hydrocarbon Fluids at Reservoir Conditions Modeling and Measurements**

**General information**
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering
Authors: Zeberg-Mikkelsen, C. K. (Intern), Stenby, E. H. (Intern)
Publication date: Sep 2001

**Publication information**
Original language: English
Main Research Area: Technical/natural sciences
Electronic versions:
40961_KT2001-Claus Kjær Zeberg-Mikkelsen-Viscosity Study of Hydrcarbon Fluids at Reservoir Conditions Modeling and Measurements.pdf
Source: orbit
Source-ID: 40961
Publication: Research › Ph.D. thesis – Annual report year: 2001

**A Thermodynamic Model for Gas Hydrates in the Presence of Salts and Methanol**

**General information**
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Zuo, Y. (Ekstern), Zhang, D. (Ekstern), Stenby, E. H. (Intern)
Pages: 175-192
Publication date: 2001
Main Research Area: Technical/natural sciences

**Publication information**
Journal: Chemical Engineering Communications
Volume: 184
ISSN (Print): 0098-6445
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.28 SJR 0.338 SNIP 0.803
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.383 SNIP 0.829 CiteScore 1.28
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.404 SNIP 0.791 CiteScore 1.2
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.411 SNIP 0.729 CiteScore 1.05
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.404 SNIP 0.813 CiteScore 1.15
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.421 SNIP 0.646 CiteScore 1.01
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.423 SNIP 0.566
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.337 SNIP 0.519
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.369 SNIP 0.535
Scopus rating (2007): SJR 0.313 SNIP 0.365
Scopus rating (2006): SJR 0.249 SNIP 0.553
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 0.345 SNIP 0.498
A Wax Inhibition Solution to Problematic Fields: A Chemical Remediation Process

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Groffe, D. (Ekstern), Groffe, P. (Ekstern), Takhar, S. (Ekstern), Andersen, S. I. (Intern), Stenby, E. H. (Intern), Lindeloff, N. (Ekstern)
Pages: 205-217
Publication date: 2001
Main Research Area: Technical/natural sciences

Publication information
Journal: Petroleum Science and Technology
Volume: 19
Issue number: 1
ISSN (Print): 1091-6466
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 0.285 SNIP 0.508 CiteScore 0.6
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.265 SNIP 0.584 CiteScore 0.48
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.296 SNIP 0.774 CiteScore 0.4
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.411 SNIP 0.851 CiteScore 0.48
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.271 SNIP 0.565 CiteScore 0.38
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.322 SNIP 0.637 CiteScore 0.5
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.27 SNIP 0.439
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.362 SNIP 0.544
BFI (2008): BFI-level 1
Density and viscosity of the 1-methylnaphthalene+2,2,4,4,6,8,8-heptamethylnonane system from 293.15 to 353.15 K at pressures up to 100 Mpa

**General information**
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Phase Equilibria and Separation Processes, Center for Energy Resources Engineering
Authors: Canet, X. (Ekstern), Dauge, P. (Ekstern), Baylaucq, A. (Ekstern), Boned, C. (Ekstern), Zeberg-Mikkelsen, C. K. (Intern), Quiñones-Cisneros, S. E. (Ekstern), Stenby, E. H. (Intern)
Pages: 1669-1689
Publication date: 2001
Main Research Area: Technical/natural sciences

**Publication information**
Journal: International Journal of Thermophysics
Volume: 22
Issue number: 6
ISSN (Print): 0195-928X
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 0.332 SNIP 0.65 CiteScore 0.83
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.39 SNIP 0.979 CiteScore 0.9
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.466 SNIP 1.104 CiteScore 1.02
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.401 SNIP 1.311 CiteScore 1.13
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
**Development of Petroleum Enhanced Coal Tar Pitch in Europe**

**General information**

State: Published

Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering


Pages: 565-572

Publication date: 2001

**Host publication information**

Title of host publication: TMS Annual Meeting, New Orleans, Louisiana, February, 2001

Main Research Area: Technical/natural sciences


Source: orbit

Source-ID: 40998

Publication: Research › Conference abstract in proceedings – Annual report year: 2001

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**Estimation of VLE Phase Compositions of Binary Systems Containing Gaseous Components, from the Feed Composition and the Cell Volume**

**General information**

State: Published

Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
High-pressure measuring cell for Raman spectroscopic studies of natural gas

A system for obtaining Raman spectra of gases at high pressure has been constructed. In order to ensure that a natural gas sample is totally representative, a high-pressure gas-measuring cell has been developed, built up by stainless steel fittings and a sapphire tube. The design and construction of this cell are described. A perfect pressure seal has been demonstrated up to 15.0 MPaA (MPa absolute). The cell has been successfully used to obtain Raman spectra of natural gas samples. Some of these spectra are presented and assigned. The most remarkable observation in the spectra is that it is possible to detect hydrogen sulfide at concentrations of 1-3 mg H2S/Nm³. An attempt to make a quantitative analysis of natural gas by the so-called "ratio method" is presented. In addition to this, the relative normalized differential Raman scattering cross sections for ethane and i-butane molecules at 8.0 MPaA and 10.2 MPaA have been determined.
High Pressure Viscosity and Density Behaviour of Ternary Mixtures: 1-Methylnaphthalene + n-Tridecane + 2,2,4,4,6,8,8-Heptamethylnonane

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Zeberg-Mikkelsen, C. K. (Intern), Canet, X. (Ekstern), Baylaucq, A. (Ekstern), Cisneros, S. (Intern), Boned, C. (Ekstern), Stenby, E. H. (Intern)
Pages: 1691-1726
Publication date: 2001
Main Research Area: Technical/natural sciences

Publication information
Journal: International Journal of Thermophysics
Volume: 22
Issue number: 6
ISSN (Print): 0195-928X
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 0.332 SNIP 0.65 CiteScore 0.83
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.39 SNIP 0.979 CiteScore 0.9
Novel Applications of Thermodynamics with Classical Models

General information
State: Published
Organisations: Department of Applied Chemistry, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Lindvig, T. (Intern), Derawi, S. (Intern), Hansen, C. (Intern), Michelsen, M. L. (Intern), Stenby, E. H. (Intern), Kontogeorgis, G. (Intern)
Publication date: 2001

Host publication information
Title of host publication: 3. Greek Scientific Conference of Chemical Engineering, Athens,
Main Research Area: Technical/natural sciences
Conference: 3. Greek Scientific Conference of Chemical Engineering, Athens, Greece, 01/01/2001
Fluid Phase Equilibria 194-197 (2002) p 663-673
Source: orbit
Source-ID: 41002
On the Mass Balance of Asphaltene Precipitation

In the evaluation of experimental data as well as in calculation of phase equilibria the necessity of the application of mass balances is obvious. In the case of asphaltenes the colloidal nature of these compounds may highly affect the mass balance. In the present paper several experiments are performed in order to check the consistency of mass balances within asphaltene precipitation. Asphaltenes are precipitated in two step processes either by changing temperature or by changes in precipitant with increasing precipitation power. This has been performed for three different oils. The data indicates that in temperature experiments as well as in solvent series experiments the precipitation of heavy asphaltenes affects the following precipitation of lighter asphaltenes. In both cases the mass balance using standard separation techniques cannot be closed, as less material is precipitated in a two step process than in the direct process either at low temperature or by direct precipitation with one precipitant. The different fractions were subject to HPLC size exclusion chromatography showing that the material remaining in solution in the stepwise process was of low molecular weight, and that the material in the second precipitation step was often of higher apparent molecular weight and had an increased overall absorbance coefficient.
Prediction of the Surface Tension of Hydrocarbons and Their Mixtures

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Phase Equilibria and Separation Processes, Center for Energy Resources Engineering
Authors: Queimada, A. (Intern), Coutinho, J. (Intern), Marrucho, I. M. (Ekstern), Kontogeorgis, G. (Intern), Stenby, E. H. (Intern)
Publication date: 2001

Host publication information
Title of host publication: Chempor 2001
Main Research Area: Technical/natural sciences
Conference: Chempor 2001 - 8th International Conference in chemical Engineering, Aveiro, Portugal, 01/01/2001
Source: orbit
Source-ID: 209312
Publication: Research - peer-review › Article in proceedings – Annual report year: 2001

Raman Spectroscopic Studies of Methane-Ethane Mixtures as a Function of Pressure
Raman spectra of methane and methane-ethane mixtures (100, 85, and 49 mole % CH4) have been obtained as a function of pressure in the pressure range 0.1 to 15.3 MPa (MPa absolute). For these mixtures methane ν1 (1)
(symmetric C-H stretching) band positions are given as a function of pressure; for pure methane they are in agreement with previous results. The new data on the methane ν₁ band position of ethane-containing mixtures clearly depend on the kind of molecules surrounding the vibrating methane molecule. The ν₁ band position decreases with increasing pressure; the stronger the dependency, the higher the content of ethane. The ethane ν₁ band position in the two mixtures showed the same kind of dependency. A qualitative explanation for this behavior is attempted, relating it to changes in van der Waals-type interactions on pressure.
Review of WAG Field Experience

In recent years there has been an increasing interest in water-alternating-gas (WAG) processes, both miscible and immiscible. WAG injection is an oil recovery method initially aimed to improve sweep efficiency during gas injection. In some recent applications produced hydrocarbon gas has been reinjected in water-injection wells with the aim of improving oil recovery and pressure maintenance. Oil recovery by WAG injection has been attributed to contact of unswept zones, especially recovery of attic or cellar oil by exploiting the segregation of gas to the top or the accumulating of water toward the bottom. Because the residual oil after gasflooding is normally lower than the residual oil after waterflooding, and three-phase zones may obtain lower remaining oil saturation, WAG injection has the potential for increased microscopic displacement efficiency. Thus, WAG injection can lead to improved oil recovery by combining better mobility control and contacting unswept zones, and by leading to improved microscopic displacement.

This study is a review of the WAG field experience as it is found in the literature today,(1-108) from the first reported WAG injection in 1957 in Canada to the new experience from the North Sea. About 60 fields have been reviewed. Both onshore and offshore projects have been included, as well as WAG injections with hydrocarbon or nonhydrocarbon gases. Well spacing is very different from onshore projects, where fine patterns often are applied, to offshore projects, where well spacing is in the order of 1000 m.

For the fields reviewed, a common trend for the successful injections is an increased oil recovery in the range of 5 to 10% of the oil initially in place (OIIP). Very few field trials have been reported as unsuccessful, but operational problems are often noted. Though the injectivity and production problems are generally not detrimental for the WAG process, special attention has been given to breakthrough of injected phases (water or gas). Improved oil recovery by WAG injection is discussed as influenced by rock type, injection strategy, miscible/immiscible gas, and well spacing.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Norsk Hydro
Authors: Christensen, J. R. (Intern), Stenby, E. H. (Intern), Skauge, A. (Ekstern)
Pages: 97-106
Publication date: 2001
Conference: 1998 SPE International Petroleum Conference and Exhibition of Mexico, Villahermose, Mexico, 01/01/1998
Main Research Area: Technical/natural sciences

Publication information
Journal: SPE Reservoir Evaluation and Engineering
Volume: 4
Issue number: 2
ISSN (Print): 1094-6470
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
Size Exclusion Chromatography in the Analysis of Pitch

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Ascanius, B. E. (Intern), Malmros, O. (Ekstern), Turner, N. R. (Ekstern), Stenby, E. H. (Intern), Andersen, S. I. (Intern)
Pages: 559-564
Publication date: 2001

Host publication information
Title of host publication: TMS Annual Meeting, New Orleans, Louisiana, February, 2001
Main Research Area: Technical/natural sciences

Original language: English
DOIs:
10.2118/71203-PA
Source: orbit
Source-ID: 169420
Publication: Research - peer-review › Journal article – Annual report year: 2001
Studies of waterflooding in low-permeable chalk by use of X-ray CT scanning

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Phase Equilibria and Separation Processes, Center for Energy Resources Engineering
Authors: Mogensen, K. (Intern), Stenby, E. H. (Intern), Zhou, D. Z. (Ekstern)
Pages: 1-10
Publication date: 2001
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Petroleum Science and Engineering
Volume: 32
ISSN (Print): 0920-4105
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.56 SJR 0.764 SNIP 1.631
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.801 SNIP 1.652 CiteScore 2.38
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.692 SNIP 1.751 CiteScore 1.95
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.822 SNIP 1.901 CiteScore 1.73
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.774 SNIP 1.666 CiteScore 1.42
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.648 SNIP 1.41 CiteScore 1.29
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.746 SNIP 1.724
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.072 SNIP 1.852
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.841 SNIP 1.435
Scopus rating (2007): SJR 0.732 SNIP 1.386
Scopus rating (2006): SJR 0.92 SNIP 1.387
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 0.784 SNIP 1.052
Scopus rating (2004): SJR 0.823 SNIP 1.302
Web of Science (2004): Indexed yes
The application of Raman Spectroscopy to study of Gas Hydrates. Phase Equilibria and Separation Processes.

General information
State: Published
Organisations: Department of Chemistry, Energy and Materials, Department of Chemistry, Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering
Authors: Hansen, S. B. (Intern), Berg, R. W. (Intern), Stenby, E. H. (Intern)
Publication date: 2001
Event: Poster session presented at The IVC-SEP 2001 and at the annual meeting in the Danish Chemical Society, Skodsborg and Odense, Denmark.
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 41020
Publication: Research - peer-review › Journal article – Annual report year: 2001

The friction theory for viscosity modeling: Extension to Crude Oil Systems

In this work the one-parameter friction theory (f-theory) general models have been extended to the viscosity prediction and modeling of characterized oils. It is demonstrated that these simple models, which take advantage of the repulsive and attractive pressure terms of cubic equations of state such as the SRK, PR and PRSV, can provide accurate viscosity prediction and modeling of characterized oils. In the case of light reservoir oils, whose properties are close to those of normal alkanes, the one-parameter f-theory general models can predict the viscosity of these fluids with good accuracy. Yet, in the case when experimental information is available a more accurate modeling can be obtained by means of a simple tuning procedure. A tuned f-theory general model can deliver highly accurate viscosity modeling above the saturation pressure and good prediction of the liquid-phase viscosity at pressures below the saturation pressure. In addition, a tuned f-theory general model delivers accurate modeling of different kinds of light and heavy oils. Thus, the simplicity and stability of the f-theory general models make them a powerful tool for applications such as reservoir simulations, between others. (C) 2001 Elsevier Science Ltd. All rights reserved.

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Cisneros, S. (Intern), Zeberg-Mikkelsen, C. K. (Intern), Stenby, E. H. (Intern)
Pages: 7007-7015
Publication date: 2001
Main Research Area: Technical/natural sciences

Publication information
Journal: Chemical Engineering Science
Volume: 56
Issue number: 24
ISSN (Print): 0009-2509
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.05 SJR 1.037 SNIP 1.442
Web of Science (2016): Indexed yes
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 $\mu_i$, 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.
Viscosity Modeling of Light Gases at Supercritical Conditions Using the Friction Theory

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Zeberg-Mikkelsen, C. K. (Intern), Cisneros, S. (Intern), Stenby, E. H. (Intern)
Pages: 3848-3854
Publication date: 2001
Main Research Area: Technical/natural sciences

Publication information
Journal: I&EC Research
Volume: 40
Issue number: 17
Original language: English
Source: orbit
Source-ID: 173991
Publication: Research - peer-review › Journal article – Annual report year: 2001

Viscosity modeling of the ternary system 1-methylnaphthalene plus n-tridecane + 2,2,4,4,6,8,8-heptamethylnonane up to 100 Mpa

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Zeberg-Mikkelsen, C. K. (Intern), Canet, X. (Ekstern), Cisneros, S. (Intern), Baylaucq, A. (Ekstern), Allal, A. (Ekstern), Boned, C. (Ekstern), Stenby, E. H. (Intern)
Pages: 281-303
Publication date: 2001
Main Research Area: Technical/natural sciences

Publication information
Journal: High Pressure Research
Volume: 21
ISSN (Print): 0895-7959
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Viscosity Prediction of Hydrocarbon Mixtures Based on the Friction Theory

The application and capability of the friction theory (f-theory) for viscosity predictions of hydrocarbon fluids is further illustrated by predicting the viscosity of binary and ternary liquid mixtures composed of n-alkanes ranging from n-pentane to n-decane for wide ranges of temperature and from low to high pressures. In the f-theory viscosity predictions the SRK and the PRSV EOS have respectively been used. Further, a comparison with the widely used LBC viscosity model shows that better results are obtained with the f-theory models. The obtained AAD% is within or close to the experimental uncertainty, which is satisfactorily for most applications related to the oil industry.

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Zeberg-Mikkelsen, C. K. (Intern), Cisneros, S. (Intern), Stenby, E. H. (Intern)
Viscosity Prediction of Hydrogen + Natural Gas Mixtures (Hythane)

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Zeberg-Mikkelsen, C. K. (Intern), Cisneros, S. (Intern), Stenby, E. H. (Intern)
Pages: 2966-2970
Publication date: 2001
Main Research Area: Technical/natural sciences

Publication information
Journal: I&EC Research
Volume: 40
Issue number: 13
Original language: English
Source: orbit
Source-ID: 40995
Publication: Research - peer-review › Journal article – Annual report year: 2001

Compositional Analysis of North Sea Oils
The molar fluid composition of either the reservoir fluid or the well stream is determined by combining the true boiling point (TBP) distillation data with gas chromatographic (GC) analysis of the light ends. For the purpose of thermodynamic simulation of phase behavior of petroleum reservoir fluids, in addition to the compositional data, physical properties of the pseudo fractions, i.e. density and molecular weight are required. A major drawback of the TBP distillation is the fact that the fractions contain typically 20 - 30% of the material outside the defined boiling range. Another significant issue is the use of generalized density and molecular weight data in the absence of experimentally determined values. This can introduce major inaccuracies in the phase behavior calculations because the generalized value of density and molecular weight significantly differ in each oil based on the paraffin-naphthene-aromatic distribution and its geographic origin.

In this work we have performed the true TBP distillation of 7 stabilized North Sea oil samples. All the oils were distilled from carbon number 6 to 19 and the distillation was terminated at C20+, which was termed as the residue. We have performed analysis of the Clo fraction of each oil by gas chromatography. Subsequently, the specific gravity and molecular weights of the TBP fractions were determined and compared with the generalized values, which indicated major differences. In addition, the superiority of the PVT calculations for a volatile oil and a gas condensate using the experimentally determined specific gravity and molecular weight of the pseudo fractions against the generalized properties is also demonstrated.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Phase Equilibria and Separation Processes, Center for Energy Resources Engineering
Authors: Dandekar, A. (Intern), Andersen, S. I. (Intern), Stenby, E. H. (Intern)
Pages: 975-988
Publication date: 2000
Main Research Area: Technical/natural sciences

Publication information
Journal: Petroleum Science and Technology
Volume: 18
Issue number: 7-8
ISSN (Print): 1091-6466
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 0.285 SNIP 0.508 CiteScore 0.6
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.265 SNIP 0.584 CiteScore 0.48
Determination of Methyl Tertiary Butyl Ether (MTBE) in Gasoline by Raman Spectroscopy

General information
State: Published
Organisations: Department of Chemistry, Department of Chemical and Biochemical Engineering
Authors: Hansen, S. B. (Intern), Berg, R. W. (Intern), Stenby, E. H. (Intern)
Pages: 65-74
Publication date: 2000
Main Research Area: Technical/natural sciences

Publication information
Journal: Asian Chemistry Letters
Volume: 4
Issue number: 1-2
ISSN (Print): 0971-9822
Ratings:
BFI (2018): BFI-level 1
Effective Algorithms for the Study of Miscible Gas Injection Processes

**General information**
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Phase Equilibria and Separation Processes
Authors: Jessen, K. (Intern), Stenby, E. H. (Intern), Michelsen, M. L. (Intern)
Number of pages: 162
Publication date: 2000

**Publication information**
ISBN (Print): 87-90142-53-5
Original language: English
Main Research Area: Technical/natural sciences
Electronic versions:
Kristian Jessen, ph.d..pdf
Source: orbit
Source-ID: 176736
Publication: Research - peer-review › Journal article – Annual report year: 2000

Effect of Low Permeable Porous Media on Behavior of Gas Condensate

**General information**
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Shapiro, A. (Intern), Potsch, K. (Ekstern), Kristensen, J. G. (Intern), Stenby, E. H. (Intern)
Publication date: 2000
Main Research Area: Technical/natural sciences

**Publication information**
Journal: SPE journal
Volume: 65182
ISSN (Print): 1086-055X
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 0.95 SNIP 2.003 CiteScore 3.01
Effect of low permeable porous media on behavior of gas condensates

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering
Authors: Shapiro, A. (Intern), Potsch, K. (Ekstern), Kristensen, J. G. (Intern), Stenby, E. H. (Intern)
Pages: 595-602
Publication date: 2000

Host publication information
Title of host publication: Proceedings of the European Petroleum Conference
Main Research Area: Technical/natural sciences
Source: orbit
Effects of Numerical Dispersion in FD Simulation of 1D Gas Injection Problems

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Jessen, K. (Ekstern), Stenby, E. H. (Intern)
Publication date: 2000
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 209292
Publication: Research - peer-review › Article in proceedings – Annual report year: 2000

Factorization of Transport Coefficients in Macroporous Media
We prove the fundamental theorem about factorization of the phenomenological coefficients for transport in macroporous media. By factorization we mean the representation of the transport coefficients as products of geometric parameters of the porous medium and the parameters characteristic of the multicomponent fluid saturating the porous space. The two permeabilities of the porous medium, the convective and the diffusional ones, are separated. A similarity between the diffusional permeability and the porosity-tortuosity factor of the Kozeny-Carman theory is demonstrated. We do not make any specific assumption about stochastic or deterministic structure of the porous medium. The fluxes in fluid on the pore level are described by general relations of the non-equilibrium thermodynamics.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering
Authors: Shapiro, A. (Intern), Stenby, E. H. (Intern)
Pages: 305-323
Publication date: 2000
Main Research Area: Technical/natural sciences
Heat Treatment in the Manufacture of Pitch Produced from Blends of Tars of Petroleum and Coal Origin

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Hansen, B. E. (Ekstern), Malmros, O. (Ekstern), Turner, N. R. (Ekstern), Stenby, E. H. (Intern), Andersen, S. I. (Intern)
Publication date: 2000
Event: Abstract from EUROCARBON 2000, 1st World Conference on Carbon, .
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 173949
Publication: Research - peer-review › Journal article – Annual report year: 2000

Including Capillary Pressure in Simulations of Steady State Relative Permeability Experiments

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Phase Equilibria and Separation Processes, Center for Energy Resources Engineering
Authors: Poulsen, S. (Intern), Skauge, T. (Ekstern), Dyrhol, S. O. (Ekstern), Stenby, E. H. (Intern), Skauge, A. (Ekstern)
Publication date: 2000

Host publication information
Title of host publication: SCA 2000-14
Main Research Area: Technical/natural sciences
Conference: the 2000 International Symposium on the Society of Core Analysts, 01/01/2000
Isothermal Gravitational Segregation: Algorithms and Specifications

New algorithms for calculating the isothermal equilibrium state of reservoir fluids under the influence of gravity are presented. Two types of specifications are considered: the specification of pressure and composition at a reference depth; and the specification of the total overall content of the reservoir, along with the reservoir geometry. It is shown how both types of calculations can be performed in an efficient and robust manner using volume-based thermodynamics. The new method makes it possible to evaluate the influence of reservoir geometry and gravity segregation on the hydrocarbon reserves. (C) 2000 Elsevier Science B.V. All rights reserved.
Low Temperature Treatment of Petroleum Tar in the Production of Anode Binder Pitch

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Hansen, B. E. (Ekstern), Malmros, O. (Ekstern), Turner, N. R. (Ekstern), Stenby, E. H. (Intern), Andersen, S. I. (Intern)
Publication date: 2000
Event: Abstract from 2nd International Conference on Petroleum and Gas Phase Behaviour, Copenhagen, Denmark.
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 209293
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2000

Measurement of Phase Boundaries of Hydrocarbon Mixtures Using Fiber Optical Detection Techniques

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Phase Equilibria and Separation Processes, Center for Energy Resources Engineering
Authors: Dandekar, A. (Intern), Stenby, E. H. (Intern)
Pages: 2586-2591
Publication date: 2000
Main Research Area: Technical/natural sciences
Publication information
Journal: Industrial & Engineering Chemistry Research
Volume: 39
Issue number: 7
ISSN (Print): 0888-5885
Ratings:
Modeling and Simulation of Nitrogen Injection in a Naturally Fractured Reservoir

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Phase Equilibria and Separation Processes, Center for Energy Resources Engineering
Authors: Jákupsstovu, S. I. (Intern), Quiñones-Cisneros, S. E. (Ekstern), Stenby, E. H. (Intern)
Publication date: 2000
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 209280
Publication: Research › Conference abstract for conference – Annual report year: 2000

Modeling of Characterized Oils Viscosity with the One Parameter Friction Theory Models

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Quiñones-Cisneros, S. E. (Ekstern), Zéberg-Mikkelsen, C. K. (Ekstern), Stenby, E. H. (Intern)
Publication date: 2000
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 209290
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2000

Models for Surfactant Systems

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Phase Equilibria and Separation Processes, Center for Energy Resources Engineering
Authors: Cheng, H. (Intern), Kontogeorgis, G. (Intern), Stenby, E. H. (Intern)
Publication date: 2000
Publication information
Publisher: Internal Report
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 209279
Publication: Research › Report – Annual report year: 2000

Raman spectroscopic studies of gasoline

General information
State: Published
Organisations: Department of Chemistry, Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering
Authors: Hansen, S. B. (Intern), Berg, R. W. (Intern), Stenby, E. H. (Intern)
Pages: 18-20, 22-23
Publication date: 2000
Main Research Area: Technical/natural sciences
Publication information
Journal: Dansk Kemi
Volume: 81
Issue number: 11
Recommended Viscosity Data and Models: \textit{n}-Alkanes

**General information**

State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Phase Equilibria and Separation Processes, Center for Energy Resources Engineering
Authors: Zeberg-Mikkelsen, C. K. (Intern), Cisneros, S. (Intern), Stenby, E. H. (Intern)
Publication date: 2000

**Publication information**

Publisher: EVIDENT Report
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 176748
Publication: Research › Journal article – Annual report year: 2000

**Recommended Viscosity Data and Models: \textit{n}-Alkanes**

**General information**

State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Phase Equilibria and Separation Processes, Center for Energy Resources Engineering
Authors: Zeberg-Mikkelsen, C. K. (Intern), Cisneros, S. (Intern), Stenby, E. H. (Intern)
Publication date: 2000

**Publication information**

Publisher: EVIDENT Report
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 176748
Publication: Research › Journal article – Annual report year: 2000

**Solid Organic Deposition During Gas Injection Studies**

Recently a series of first contact miscibility (swelling) experiments have been performed on undersaturated light and heavy oils using LPG rich and methane rich injection gases, in which solid organic deposition was observed. A compositional gradient in the oils during the gas injection process was also evident as oil fractions expelled from the top to bottom of the PVT cell were observed to vary in density, molecular weight, as well as darkness of color. The change in stability of the oil samples before and after the contact with gas was analyzed using flocculation threshold titration. The asphaltene content of the different oil samples were determined by the TP 143 method. The standard asphaltenes and the solid organic deposit recovered from the swelling tests were analyzed using FTIR, HPLC-SEC and H-1 NMR. The aim of these analyses is to reveal the molecular nature of the deposits formed during the gas injection process in comparison with the standard asphaltenes in order to understand the mechanisms involved in asphaltene deposition.

**General information**

State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Phase Equilibria and Separation Processes, Center for Energy Resources Engineering
Authors: Dandekar, A. Y. (Ekstern), Andersen, S. I. (Intern), Stenby, E. H. (Intern)
Pages: 1209-1229
Publication date: 2000
Main Research Area: Technical/natural sciences

**Publication information**

Publisher: Petroleum Science and Technology
Volume: 18
Issue number: 9-10
ISSN (Print): 1091-6466
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 0.285 SNIP 0.508 CiteScore 0.6
BFI (2015): BFI-level 1
The Application of Raman Spectroscopy for Analysis of Multi-Component Systems

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Department of Chemistry, Center for Phase Equilibria and Separation Processes
Authors: Hansen, S. B. (Intern), Berg, R. W. (Intern), Stenby, E. H. (Intern)
Publication date: 2000

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Electronic versions:
Susanne Brunsgaard Hansen, ph.d..pdf
Source: orbit
Source-ID: 192276
The Friction Theory (f-theory) for Viscosity Modeling

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering
Authors: Cisneros, E. S. P. (Intern), Zeberg-Mikkelsen, C. K. (Intern), Stenby, E. H. (Intern)
Pages: 249-276
Publication date: 2000
Main Research Area: Technical/natural sciences

Publication information
Journal: Fluid Phase Equilibria
Volume: 169
ISSN (Print): 0378-3812
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 2.33 SJR 0.869 SNIP 1.155
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.874 SNIP 0.998 CiteScore 1.99
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 0.982 SNIP 1.248 CiteScore 2.28
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.007 SNIP 1.274 CiteScore 2.31
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.152 SNIP 1.286 CiteScore 2.31
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.034 SNIP 1.234 CiteScore 2.26
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 0.986 SNIP 1.317
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.133 SNIP 1.164
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.227 SNIP 1.09
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.031 SNIP 1.151
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.034 SNIP 1.245
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.009 SNIP 1.3
Comparison of Iterative Methods for Computing the Pressure Field in a Dynamic Network Model

In dynamic network models, the pressure map (the pressure in the pores) must be evaluated at each time step. This calculation involves the solution of a large number of nonlinear algebraic systems of equations and accounts for more than 80 of the total CPU-time. Each nonlinear system requires at least the partial solution of a sequence of linear systems. We present a comparative study of iterative methods for solving these systems, where we apply both standard routines from the public domain package ITPACK 2C and our own routines tailored to the network problem. The conjugate gradient method, preconditioned by symmetric successive overrelaxation, was found to be consistently faster and more robust than the other solvers tested. In particular, it was found to be much superior to the successive overrelaxation technique currently used by many researchers.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Department of Informatics and Mathematical Modeling, Mærsk Olie og Gas A/S, S.N. Bose National Center for Basic Sciences
Authors: Mogensen, K. (Ekstern), Stenby, E. H. (Intern), Banerjee, S. (Ekstern), Barker, V. A. (Intern)
Pages: 277-301
Publication date: 1999
Main Research Area: Technical/natural sciences

Publication information
Journal: Transport in Porous Media
Volume: 37
Issue number: 3
ISSN (Print): 0169-3913
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.16 SJR 0.767 SNIP 1.316
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.728 SNIP 1.317 CiteScore 1.94
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.932 SNIP 1.433 CiteScore 1.91
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.04 SNIP 1.433 CiteScore 2.03
ISI indexed (2013): ISI indexed yes
Fast, Approximate Solutions for 1D Multicomponent Gas Injection Problems

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering
Authors: Jessen, K. (Intern), Wang, Y. (Ekstern), Ermakov, P. (Ekstern), Zhu, J. (Ekstern), Orr Jr, F. (Ekstern), Stenby, E. H. (Intern)
Publication date: 1999

Host publication information
Title of host publication: Fast, Approximate Solutions for 1D Multicomponent Gas Injection Problems
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 174947
Publication: Research - peer-review › Book chapter – Annual report year: 1999

Forbedring af olieindvinding ved gasinjektion

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Phase Equilibria and Separation Processes
High Pressure Multicomponent Adsorption in Porous Media

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering
Authors: Shapiro, A. (Intern), Stenby, E. H. (Intern)
Pages: 565-573
Publication date: 1999
Main Research Area: Technical/natural sciences

Publication information
Journal: Fluid Phase Equilibria
Volume: 158-160
ISSN (Print): 0378-3812
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 2.33 SJR 0.869 SNIP 1.155
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.874 SNIP 0.998 CiteScore 1.99
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 0.982 SNIP 1.248 CiteScore 2.28
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.007 SNIP 1.274 CiteScore 2.31
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.152 SNIP 1.286 CiteScore 2.31
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes

Authors: Jessen, K. (Intern), Stenby, E. H. (Intern)
Pages: 35-36
Publication date: 1999
Main Research Area: Technical/natural sciences

Publication information
Journal: Dansk Kemi
Volume: 80
Issue number: (5)
ISSN (Print): 0011-6335
Ratings:
ISI indexed (2013): ISI indexed no
ISI indexed (2012): ISI indexed no
ISI indexed (2011): ISI indexed no
Web of Science (2007): Indexed yes
Web of Science (2004): Indexed yes
Original language: Danish
Source: orbit
Source-ID: 174796
Publication: Research › Journal article – Annual report year: 1999
High Pressure Wax Formation

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, University of Pau and Pays de l'Adour
Authors: Lindeloff, N. (Intern), Andersen, S. I. (Intern), Pauly, J. (Ekstern), Daridon, J. (Ekstern), Stenby, E. H. (Intern)
Publication date: 1999

Host publication information
Title of host publication: High Pressure Wax Formation
Main Research Area: Technical/natural sciences
Conference: 1999 AIChE National Spring Meeting, Houston, TX, United States, 14/03/1999 - 14/03/1999
Source: orbit
Source-ID: 170989
Publication: Research - peer-review › Journal article – Annual report year: 1999

Modelling of Aggregation Behavior and Precipitation for Asphaltene-Containing Fluids

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, St. Petersburg State University
Authors: Andersen, S. I. (Intern), Victotov, A. (Ekstern), Stenby, E. H. (Intern)
Nonequilibrium Segregation in Petroleum Reservoirs

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering
Authors: Shapiro, A. (Intern), Stenby, E. H. (Intern)
Pages: 55-60
Publication date: 1999
Conference: IMT3 Third International Meeting on Thermodiffusion, Mons, Belgium, 01/01/1998
Main Research Area: Technical/natural sciences

Phase-Boundary Calculations in Systems Involving More than Two Phases, with Application to Hydrocarbon Mixtures

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, University of Calgary
Authors: Lindeloff, N. (Intern), Heidemann, R. (Ekstern), Andersen, S. I. (Intern), Stenby, E. H. (Intern)
Pages: 1107-1113
Publication date: 1999
Main Research Area: Technical/natural sciences
Predicting the Melting Points and the Heats of Fusion of Saturated Triglycerides by a Group Contribution Method

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering
Authors: Zeberg-Mikkelsen, C. (Ekstern), Stenby, E. H. (Intern)
Pages: 7-17
Publication date: 1999
Main Research Area: Technical/natural sciences

Publication information
Journal: Fluid Phase Equilibria
Volume: 162
ISSN (Print): 0378-3812
Ratings:
BFI (2018): BFI-level 2
A Dynamic Pore-Scale Model of Imbibition

We present a dynamic pore-scale network model of imbibition, capable of calculating residual oil saturation for any given capillary number, viscosity ratio, contact angle and aspect ratio. Our goal is not to predict the outcome of core floods, but rather to perform a sensitivity analysis of the above-mentioned parameters, except the viscosity ratio. We find that contact angle, aspect ratio and capillary number all have a significant influence on the competition between piston-like advance, leading to high recovery, and snap-off, causing oil entrapment. Due to enormous CPU-time requirements we could not incorporate long-range correlations among pore and throat sizes in our network, but were limited to small-range correlations. Consequently, the gradual suppression of snap-off occurs within one order of magnitude of the capillary number. At capillary numbers around 10^-5 to 10^-4, snap-off has been entirely inhibited, in agreement with results obtained by Blunt using a quasi-static model. For higher aspect ratios, the effect of rate and contact angle is more pronounced. Many core floods are conducted at capillary numbers in the range 10 to 10^-6. We believe that the excellent recoveries observed during our waterfloods on tight chalk may be explained by the combined effect of rate, non-zero contact angle and existence of long-range correlations. Vast reductions in residual oil saturations are largely due to suppression of snap-off in favour of frontal displacement, whereas ganglion mobilization plays a much more modest role in the displacement of continuous oil.

P. 47
A Dynamic Two-Phase Pore-Scale Model of Imbibition

We present a dynamic pore-scale network model of imbibition, capable of calculating residual oil saturation for any given capillary number, viscosity ratio, contact angle, and aspect ratio. Our goal is not to predict the outcome of core floods, but rather to perform a sensitivity analysis of the above-mentioned parameters, except from the viscosity ratio. We find that contact angle, aspect ratio, and capillary number all have a significant influence on the competition between piston-like advance, leading to high recovery, and snap-off, causing oil entrapment. Due to significant CPU-time requirements we did not incorporate long-range correlations among pore and throat sizes in our network, but were limited to small-range correlations. Consequently, the gradual suppression of snap-off occurs within one order of magnitude of the capillary number. At capillary numbers around 10^{-8}-10^{-7}, snap-off has been entirely inhibited, in agreement with results obtained by Blunt (1997) who used a quasi-static model. For higher aspect ratios, the effect of rate and contact angle is more pronounced.
Analysis of Multicomponent Adsorption Close to a Dew Point

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering
Authors: Shapiro, A. (Intern), Stenby, E. H. (Intern)
Pages: 546-557
Publication date: 1998
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Colloid and Interface Science
Volume: 206
ISSN (Print): 0021-9797
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 4.14 SJR 1.144 SNIP 1.267
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.095 SNIP 1.263 CiteScore 3.8
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.166 SNIP 1.406 CiteScore 3.74
Web of Science (2014): Indexed yes
A simple model for the prediction of asphaltene precipitation is proposed. The model is based on an equation of state and uses standard thermodynamics, thus assuming that the precipitation phenomenon is a reversible process. The solid phase is treated as an ideal multicomponent mixture. An activity coefficient model based on the athermal Flory-Huggins expression was included to account for solid phase non-ideality, but was found to have little effect on the results. Only a fraction of each of the heaviest components are considered potentially solid forming. This approach is based on the assumption, that out of the total PNA composition of a crude, the asphaltenes and resins are mainly aromatic-naphtenic in their nature. The predictions shows the correct qualitative behavior with respect to temperature and pressure, but due to lack of data the model was not evaluated quantitatively with respect to these effects.
Calculation of Interfacial Tensions of Hydrocarbon-water Systems under Reservoir Conditions

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, D.B. Robinson Research Ltd.
Authors: Zuo, Y. (Ekstern), Stenby, E. H. (Intern)
Pages: 157-180
Publication date: 1998
Main Research Area: Technical/natural sciences

Publication information
Journal: In Situ
Volume: 22
Issue number: 2
Original language: English
Source: orbit
Source-ID: 169418

Compositional and Relative Permeability Hysteresis Effects on Near-Miscible WAG
Evaluation of compositional effects and fluid flow description on near-miscible (water-alternating-gas) WAG modeling have been studied for a North Sea oil field starting production in 1998. A sector model with four wells was applied to simulate a heterogeneous sandstone reservoir, and a compositional model was used to compare different production strategies e.g. waterflooding and a near-miscible (WAG) injection. In the WAG scheme both dry and wet (rich) hydrocarbon gases have been considered for injection. The phase behaviour was quantified by comparing the performance of the different injection gases.

Result obtained shows the WAG injection gives improved recovery compared to water injection, due to better sweep and lower residual oil saturation. Simulations with and without relative permeability hysteresis (two-phase model) were compared. The effect of trapped gas on oil recovery does not seem significant with the compositional model. The WAG process has been optimized with respect to slug size and the water-gas ratio.

A black-oil-model was generated tuned to fit the results from the compositional simulations. A WAG three-phase relative permeability hysteresis model using cycle dependent relative permeabilities for both wetting and non-wetting phases, have been compared to the standard two-phase Killough and Carlson hysteresis models. The results show significant lower gas ratio and a higher oil recovery for the WAG injection when using cycle dependent relative permeabilities.

The simulations show sensitivity toward the three-phase model whereas Carlsen/Killough type hysteresis has little/no influence on the oil recovery.

Simulations indicates that the recovery by WAG-injection may be underestimated in the compositional model due to lack of possibility for cycle dependent relative permeability hysteresis, whereas the black oil model underestimates the phase behaviour effect. The results indicate that the WAG-injection might have an upside potential with respect to the influence of combined phase behaviour and relative permeability effects.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Norsk Hydro
Authors: Christensen, J. R. (Intern), Stenby, E. H. (Intern), Skauge, A. (Ekstern)
Pages: 233-248
Publication date: 1998

Host publication information
Title of host publication: Proceedings of the SPE/DOE Improved Oil Recovery Symposium
Publisher: Society of Petroleum Engineers
ISBN (Print): 978-1-55563-387-5
Main Research Area: Technical/natural sciences
Conference: SPE/DOE Improved Oil Recovery Symposium, April 18-24, Tulsa, Oklahoma, 01/01/1998
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10.2118/39627-MS
Source: orbit
Source-ID: 176071
Effective Algorithm for Calculation of Minimum Miscibility Pressure

This paper describes a new algorithm developed for calculation of the minimum miscibility pressure (MMP) for the displacement of oil by a multicomponent injection gas. The algorithm is based on the key tie line identification approach initially studied by Wang and Orr [Y. Wang and F.M. Orr Jr., Analytical calculation of minimum miscibility pressure, Fluid Phase Equilibria, 139 (1997) 101-124]. A new global formulation is introduced to describe and locate the sequence of \( n_c - 1 \) key tie lines controlling the development of miscibility. In this new formulation, a number of numerical weaknesses of the original approach have been eliminated resulting in a robust and highly efficient algorithm. The computation time is reduced significantly and is clearly superior to other methods described in the literature. For a 15 component fluid description the MMP is determined within a few seconds on a PC. Hence the algorithm offers an efficient tool for projects where a large number of MMP calculations are needed (e.g. lumping and gas enrichment studies).

A case study is presented based on a real reservoir fluid for which PVT studies, swelling test and slimtube experiments have been performed. The study aims at investigating the influence of the characterization, tuning and lumping procedure used for generating a fluid description on the prediction of the MMP.

Based on the generated fluid description, a gas enrichment study is presented where the optimum mixture of two available injection gasses is determined aiming to optimize the gas injection project.

Global Approach for Calculation of Minimum Miscibility Pressure

An algorithm has been developed for calculation of minimum miscibility pressure (MMP) for the displacement of oil by multicomponent gas injection. The algorithm is based on the key tie line identification approach initially addressed by Wang and Orr [Y. Wang and F.M. Orr Jr., Analytical calculation of minimum miscibility pressure, Fluid Phase Equilibria, 139 (1997) 101-124]. In this work a new global approach is introduced. A number of deficiencies of the sequential approach have been eliminated resulting in a robust and highly efficient algorithm. The time consumption for calculation of the MMP in multicomponent displacement processes has been reduced significantly and can now be performed within a few seconds on a PC for a 15-component gas mixture. The algorithm is hence particularly suitable for gas enrichment studies or other case studies where a large number of MMP calculations is required. Predicted results from the key tie line identification approach are shown to be in excellent agreement with slimtube data and with other multicell/slimtube simulators presented in the literature.
gas injection, vapor-liquid equilibria, minimum miscibility pressure (MMP), multicomponent mixtures, efficient method of calculation
Investigation of Asphaltene Precipitation at Elevated Temperature

In order to obtain quantitative data on the asphaltene precipitation induced by the addition of n-alkane (heptane) at temperatures above the normal boiling point of the precipitant, a high temperature/high pressure filtration apparatus has been constructed. Oil and alkane are mixed at the appropriate temperature and the pressure in closed vessels keeping the mixture at the liquid state. The filtration is performed with a small differential pressure over the filter so as to avoid flashing the mixture. The technique requires a low dead volume in the system to minimize the content of maltenes in the extracted fraction, hence there is no room for stirring. The equipment as well as solutions to some of the problems are presented along with precipitation data from 40 to 200 degrees C. The asphaltenes separated are analyzed using FT-ir. The filtrate containing the maltenes was cooled to room temperature and the asphaltenes separating upon cooling was collected and analyzed. The oil and selected malten fractions and extraction/cleaning solvents were analyzed using GC.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering
Authors: Andersen, S. I. (Intern), Lindeloff, N. (Intern), Stenby, E. H. (Intern)
Pages: 323-334
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Conference: 2nd International Symposium on Thermodynamics of Heavy Oils and Asphaltenes, Houston, TX, United States, 09/03/1997 - 09/03/1997
Main Research Area: Technical/natural sciences

Publication information
Journal: Petroleum Science and Technology
Volume: 16
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BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 0.285 SNIP 0.508 CiteScore 0.6
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.265 SNIP 0.584 CiteScore 0.48
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.296 SNIP 0.774 CiteScore 0.4
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.411 SNIP 0.851 CiteScore 0.48
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.271 SNIP 0.565 CiteScore 0.38
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.322 SNIP 0.637 CiteScore 0.5
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.27 SNIP 0.439
BFI (2009): BFI-level 1
Measurement of Viscosity of Hydrocarbon Liquids Using a Microviscometer

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering
Authors: Dandekar, A. (Intern), Andersen, S. I. (Intern), Stenby, E. H. (Intern)
Pages: 551-554
Publication date: 1998
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Chemical and Engineering Data
Volume: 43
Original language: English
Source: orbit
Source-ID: 169419
Publication: Research - peer-review › Journal article – Annual report year: 1998

Multiphase Flow in Low-Permeable Chalk, X-Ray CT Scanning and Pore-Level Modelling

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering
Authors: Mogensen, K. (Ekstern), Stenby, E. H. (Intern)
Publication date: 1998

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 174506
Publication: Research - peer-review › Book – Annual report year: 1998
Prediction of Interfacial Tensions of Reservoir Crude Oil and Gas Condensate Systems

In this work, the linear gradient theory (LGT) model, the simplified linear gradient theory (SLGT) model, the corresponding-states (CS) correlation, and the parachor method developed by the authors were extended to calculate interfacial tensions (IFT’s) of crude oil and gas condensate systems. Correlations of the model parameters were presented for pseudocomponents. The characterization procedures of Pedersen et al. and the SRK equation of state (EOS) were used to calculate vapor-liquid equilibria (VLE). To the exclusion of the near-critical region, the IFT’s calculated by all the models except the CS correlation were in good agreement with the measured IFT data for several crude oil and CO2/oil systems. The SLGT model and the parachor model perform better than the LGT model and the CS correlation. For N 2 volatile oil systems, the performance of the LGT model is better than that of the SLGT model and the parachor model. For gas condensate systems, the predictions by use of the SLGT model are in good agreement with the measured IFT data. In the near-critical region, a correlation was proposed for estimations of IFT’s for CO2/oil systems, and satisfactory correlated results were obtained.
Ramanspektroskopisk undersøgelse af Metyltertiærbutylether indhold i benzin: MTBE

General information
State: Published
Organisations: Department of Chemistry, Department of Chemical and Biochemical Engineering
Authors: Hansen, S. B. (Intern), Berg, R. W. (Intern), Stenby, E. H. (Intern)
Number of pages: 12
Publication date: 1998

Publication information
Original language: Danish
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 170666
Publication: Research - peer-review › Report – Annual report year: 1998

Simulation of the High-Pressure Phase Equilibria of Hydrocarbonwater/Brine Systems

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering
Authors: Zuo, Y. X. (Ekstern), Stenby, E. H. (Intern)
Pages: 99-101
Publication date: 1998
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Petroleum Science and Engineering
A Percolation Study of Wettability Effect on the Electrical Properties of Reservoir Rocks

Measurements of the electrical resistivity of oil reservoirs are commonly used to estimate other properties of reservoirs, such as porosity and hydrocarbon reserves. However, the interpretation of the measurements is based on empirical correlations, because the underlying mechanisms that control the electrical properties of oil bearing rocks have not been well understood. In this paper, we employ percolation concepts to investigate the effect of wettability on the electrical conductivity of a reservoir formation. A three-dimensional simple cubic network is used to represent an ideal reservoir formation, for which the effect of the wettability can be isolated from the others. The phase distribution in the network is analyzed for different flow processes, and the conductivity is then estimated using a power law approximation of the percolation quantities.

The proposed conceptual model predicts the generic behavior of reservoir resistivities of different wettabilities. It demonstrates that the resistivity index depends on saturation history and wettability. For strongly oil-wet systems, significant hysteresis is expected, while there is little hysteresis for strongly water-wet systems, and some hysteresis is also expected for intermediate wet systems. One of the interesting results from this study is that for intermediate wet systems, Archie's saturation exponent is between 1.9 and 3.0.
Application of Raman Spectroscopy for Analysis

General information
State: Published
Organisations: Department of Chemistry, Department of Chemical and Biochemical Engineering
Authors: Hansen, S. B. (Intern), Berg, R. W. (Intern), Stenby, E. H. (Intern)
Publication date: 1997

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Title of host publication: Application of Raman Spectroscopy for Analysis
Main Research Area: Technical/natural sciences
Conference: SPE MEETING, DTU, Lyngby, Denmark, 01/01/1997
Source: orbit
Source-ID: 168284
Publication: Research - peer-review › Journal article – Annual report year: 1997

A Thermodynamic Mixed-Soiled Asphalthene Precipitation Model

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering
Authors: Lindeloff, N. (Intern), Heidemann, R. (Ekstern), Andersen, S. I. (Intern), Stenby, E. H. (Intern)
Publication date: 1997

Host publication information
Title of host publication: A Thermodynamic Mixed-Soiled Asphalthene Precipitation Model
Main Research Area: Technical/natural sciences
Conference: 2nd International Symposium on Thermodynamics of Heavy Oils and Asphaltenes, Houston, TX, United States, 09/03/1997 - 09/03/1997
Source: orbit
Source-ID: 176058
Publication: Research › Article in proceedings – Annual report year: 1997

Calculation of interfacial tensions with gradient theory. I. Pure and Pseudo-Pure Fluids. II. Binary Systems

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, D.B. Robinson Research Ltd.
Authors: Zuo, Y. (Ekstern), Stenby, E. H. (Intern)
Pages: 139-158
Publication date: 1997
Main Research Area: Technical/natural sciences

Publication information
Journal: Fluid Phase Equilibria
Volume: 132
ISSN (Print): 0378-3812
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 2.33 SJR 0.869 SNIP 1.155
Web of Science (2016): Indexed yes
Calculation of Minimum Miscibility Pressure

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering
Authors: Bleriot, L. (Ekstern), Jessen, K. (Intern), Michelsen, M. L. (Intern), Stenby, E. H. (Intern)
Corresponding-States and Parachor Models for the Calculation of Interfacial Tensions

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, D.B. Robinson Research Ltd.
Authors: Zuo, Y. (Ekstern), Stenby, E. H. (Intern)
Pages: 1130-1137
Publication date: 1997
Main Research Area: Technical/natural sciences

Publication information
Journal: Canadian Journal of Chemical Engineering
Volume: 75
ISSN (Print): 0008-4034
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.41 SJR 0.504 SNIP 0.805
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.41 SNIP 0.656 CiteScore 1.13
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.504 SNIP 0.815 CiteScore 1.28
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.476 SNIP 0.798 CiteScore 1.16
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.427 SNIP 0.813 CiteScore 0.99
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.429 SNIP 0.692 CiteScore 0.94
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.415 SNIP 0.627
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.365 SNIP 0.68
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.358 SNIP 0.481
Scopus rating (2007): SJR 0.449 SNIP 0.534
Scopus rating (2006): SJR 0.344 SNIP 0.631
Scopus rating (2005): SJR 0.428 SNIP 0.784
Scopus rating (2004): SJR 0.378 SNIP 0.629
Scopus rating (2003): SJR 0.513 SNIP 0.552
Effect of Temperature on the Precipitation and Composition of Asphaltenes

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering
Authors: Andersen, S. I. (Intern), Lindeloff, N. (Intern), Stenby, E. H. (Intern)
Publication date: 1997

Host publication information
Title of host publication: Proceedings of the 16th European Seminar on Applied Thermodynamics
Main Research Area: Technical/natural sciences
Conference: 16th European Seminar on Applied Thermodynamics, Pont-à-Mousson, France, 19/06/1997 - 19/06/1997
Source: orbit
Source-ID: 174501
Publication: Research - peer-review › Article in proceedings – Annual report year: 1997

Kelvin Equation for a Non-Ideal Multicomponent Mixture

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering
Authors: Shapiro, A. (Intern), Stenby, E. H. (Intern)
Pages: 87-101
Publication date: 1997
Main Research Area: Technical/natural sciences

Publication information
Journal: Fluid Phase Equilibria
Volume: 134
ISSN (Print): 0378-3812
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 2.33 SJR 0.869 SNIP 1.155
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.874 SNIP 0.998 CiteScore 1.99
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 0.982 SNIP 1.248 CiteScore 2.28
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.007 SNIP 1.274 CiteScore 2.31
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Measurement of Phase Behavior of Hydrocarbon Mixtures Using Fiber Optical Detection Techniques

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering
Authors: Dandekar, A. (Intern), Stenby, E. H. (Intern)
Publication date: 1997
Conference: 72nd Annual Technical Conference and Exhibition of the Society of Petroleum Engineers, San Antonio, Texas, USA, 01/01/1997
Main Research Area: Technical/natural sciences

Publication information
Journal: Unknown title
Original language: English
Source: orbit
Source-ID: 168250
Publication: Research - peer-review › Journal article – Annual report year: 1997
Prediction of Gas Hydrate Formation Conditions in Aqueous Solutions of Single and Mixed Electrolytes

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, D.B. Robinson Research Ltd.
Authors: Zuo, Y. (Ekstern), Stenby, E. H. (Intern)
Pages: 406-416
Publication date: 1997
Main Research Area: Technical/natural sciences

Publication information
Journal: SPE Journal
Volume: 2
Original language: English
Source: orbit
Source-ID: 168283
Publication: Research - peer-review › Journal article – Annual report year: 1997

Presentations of the research activities in IVC-SEP

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering
Authors: Stenby, E. H. (Intern)
Publication date: 1997

Host publication information
Title of host publication: Presentations of the research activities in IVC-SEP
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 176061
Publication: Research › Article in proceedings – Annual report year: 1997

The influence of the porous medium on the phase behavior of reservoir fluids

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering
Authors: Stenby, E. H. (Intern)
Publication date: 1997

Host publication information
Title of host publication: The influence of the porous medium on the phase behavior of reservoir fluids
Main Research Area: Technical/natural sciences
Conference: Conference on Production of Reservoir Fluids in Frontier Conditions, Ruell-Malmaison, France, 01/01/1997
Variations in Composition of Subfractions of Petroleum Asphaltenes

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering
Authors: Andersen, S. I. (Intern), Keul, A. (Ekstern), Stenby, E. H. (Intern)
Pages: 611-646
Publication date: 1997
Main Research Area: Technical/natural sciences

Publication information
Journal: Petroleum Science and Technology
Volume: 15
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Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 0.285 SNIP 0.508 CiteScore 0.6
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.265 SNIP 0.584 CiteScore 0.48
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.296 SNIP 0.774 CiteScore 0.4
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.411 SNIP 0.851 CiteScore 0.48
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.271 SNIP 0.565 CiteScore 0.38
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.322 SNIP 0.637 CiteScore 0.5
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.27 SNIP 0.439
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.362 SNIP 0.544
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.283 SNIP 0.497
Scopus rating (2007): SJR 0.265 SNIP 0.484
Scopus rating (2006): SJR 0.327 SNIP 0.46
Scopus rating (2005): SJR 0.345 SNIP 0.572
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 0.396 SNIP 0.689
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 0.311 SNIP 0.458
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 0.467 SNIP 0.581
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 0.619 SNIP 0.941
Wax Formation in Petroleum Systems-Solvent Fraction, Characterization and Thermodynamic Modelling

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering
Authors: Andersen, S. I. (Intern), Lindeloff, N. (Intern), Stenby, E. H. (Intern)
Publication date: 1997

Host publication information
Title of host publication: Wax Formation in Petroleum Systems-Solvent Fraction, Characterization and Thermodynamic Modelling
Main Research Area: Technical/natural sciences
Conference: International Symp. on Thermodynamics of Wax Formation from Petroleum, AIChE Spring Meeting, Houston, 01/01/1997
Source: orbit
Source-ID: 176068
Publication: Research › Article in proceedings – Annual report year: 1997

A Consistent Procedure for Pseudo-Component Delumping

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CFL Consulting, Haldor Topsoe AS
Authors: Leibovici, C. (Ekstern), Stenby, E. H. (Intern), Knudsen, K. (Ekstern)
Pages: 510-517
Publication date: 1996
Conference: FPPECPD, Snowmass, USA, 01/01/1996
Main Research Area: Technical/natural sciences

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Journal: Fluid Phase Equilibria
Volume: 116
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Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 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
A Linear Gradient Theory Model for Calculating Interfacial Tensions of Mixtures

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering
Authors: Zou, Y. (Ekstern), Stenby, E. H. (Intern)
Pages: 126-132
Publication date: 1996
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Colloid and Interface Science
Volume: 182
Issue number: 0443
ISSN (Print): 0021-9797
Ratings:
BFI (2018): BFI-level 1
A Local Composition Model for Paraffinic Solid Solutions

The description of the solid-phase non-ideality remains the main obstacle in modelling the solid-liquid equilibrium of hydrocarbons. A theoretical model, based on the local composition concept, is developed for the orthorhombic phase of n-alkanes and tested against experimental data for binary systems. It is shown that it can adequately predict the experimental phase behaviour of paraffinic mixtures. This work extends the applicability of local composition models to the solid phase. Copyright (C) 1996 Elsevier Science Ltd.
Application of a Delumping Procedure to Compositional Reservoir Simulations

Characterization and lumping are always performed when dealing with reservoir fluids. The number of pseudocomponents in a compositional reservoir simulation is normally between three and eight. In order to optimize the reservoir performance, it is necessary to know a detailed composition of the product stream from the reservoir. This paper deals with the problems of how to come from the lumped system (for which the reservoir simulation was performed) to a description of the full system (which is important in order to optimize the down-stream facilities). The equations of the delumping procedure are shown and the application of the method is illustrated through examples, including a constant volume depletion experiment and the fifth SPE Comparative example with a fluid description from a North Sea reservoir (with the calculated composition after a lumping, an experiment and a delumping).

Introduction

The use of reservoir simulators play an important role when planning, developing and producing almost every oil and gas field. It is accepted that the compositional simulation is a necessary tool when complicated fluid behaviour needs to be investigated accurately e.g. near critical fluids, gas condensates or gas injection processes.

A common calculation procedure is to divide the reservoir into a number of gridblocks. For each gridblock a mass balance is applied together with the iso-fugacity criteria for the phases present (oil, gas or water). The number of blocks used in full field models can be in the range from very few (20-50) up to several thousand blocks. However, due to the large amount of calculations required and the problems related with obtaining an accurate fluid description especially for the heaviest oil fraction, it is normal to simplify the fluid description by the use of pseudo-components (average components or components from characterization of the heavy oil fraction). The number of pseudo-components by most authors recommended to not less than six. In practice a number from three to eight is used.

Where a minimum of six pseudocomponents are considered reasonable for the up-stream calculations it is a far too low number for the down-stream calculations e.g. a distillation calculation will normally require detailed knowledge of 50-100 components for sufficient accuracy - particular in situations where different oils are mixed. Thus it is important to calculate detailed component information from the output of the compositional reservoir simulation. This calculation is here referred to as delumping.

One of the first delumping method proposed by Drohm et al. is based on a Gibbs energy minimization using correlation's from a previous suggested lumping procedure. Danesh et al. published a K-factor method using the acentric factor and the reduced temperature. This paper will mainly use the method suggested by Leibovici et al., which is based on the simplified flash of Michelsen.

Calculations are made to show how the delumping can be used to generate a full component description from a lumped system. Especially the aspect of using the output from a compositional reservoir simulator in a process simulator is an important application for the delumping procedure. An example of a calculation from a constant volume depletion (CVD) experiment and a reservoir simulation with the calculated composition after a lumping, an experiment and a delumping are also given.
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.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering
Authors: Coutinho, J. A. (Ekstern), Stenby, E. H. (Intern)
Pages: 918-925
Publication date: 1996
Main Research Area: Technical/natural sciences

Publication information
Journal: Industrial & Engineering Chemistry Research
Volume: 35
ISSN (Print): 0888-5885
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.1 SJR 0.945 SNIP 1.139
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.949 SNIP 1.146 CiteScore 2.87
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.012 SNIP 1.292 CiteScore 2.85
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 0.982 SNIP 1.243 CiteScore 2.6
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.066 SNIP 1.338 CiteScore 2.56
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.086 SNIP 1.24 CiteScore 2.58
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.047 SNIP 1.165
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.002 SNIP 1.164
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 1.142 SNIP 1.267
Simulation of Flow Behavior of Gas Condensate at Low Interfacial Tension

**General information**
State: Published
Organisations: Department of Chemical and Biochemical Engineering
Authors: Wang, P. (Ekstern), Stenby, E. H. (Intern), Pope, G. A. (Ekstern), Sepehrnoori, K. (Ekstern)
Pages: 199-219
Publication date: 1996
Main Research Area: Technical/natural sciences

**Publication information**
Journal: IN SITU
Volume: 20
Issue number: 2
Original language: English
Source: orbit
Source-ID: 168051
Publication: Research - peer-review › Journal article – Annual report year: 1996

Simulation of the high-pressure phase equilibria of hydrocarbon-water/brine systems

**General information**
State: Published
Organisations: Department of Chemical and Biochemical Engineering
Authors: Zuo, Y. (Ekstern), Stenby, E. H. (Intern), Guo, T. (Ekstern)
Pages: 201-220
Publication date: 1996
Main Research Area: Technical/natural sciences

**Publication information**
Journal: Journal of Petroleum Science and Engineering
Volume: 15
ISSN (Print): 0920-4105
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
Solid-Liquid equilibrium of n-alkanes using the Chain Delta Lattice Parameter model

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering
Authors: Coutinho, J. A. (Ekstern), Andersen, S. I. (Intern), Stenby, E. H. (Intern)
Pages: 138-145
Publication date: 1996
Statistical Description of Segregation in a Powder Mixture

In this paper we apply the statistical mechanics of powders to describe a segregated state in a mixture of grains of different sizes. Variation of the density of a packing with depth arising due to changes of particle configurations is studied. The statistical mechanics of powders is generalized in such a way as to consider not only binary mixtures (as its first formulation by A. Mehta and S.F. Edwards), but also polydisperse mixtures of particles.
Thermodynamics of Asphaltene Precipitation and Dissolution Investigation of Temperature and Solvent Effects

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering
Authors: Andersen, S. I. (Intern), Stenby, E. H. (Intern)
Pages: 261-287
Publication date: 1996
Main Research Area: Technical/natural sciences

Publication information
Journal: Fuel Science and Technology Int
Volume: 1
Issue number: 14(1&2)
Original language: English
Source: orbit
Source-ID: 174499
Publication: Research - peer-review › Journal article – Annual report year: 1996

Phase equilibria in petroleum fluids: multiphase regions and wax formation

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering
Authors: Coutinho, J. (Intern), Stenby, E. H. (Intern)
Number of pages: 177
Publication date: 1995

Publication information
Place of publication: Kgs.Lyngby
Publisher: Technical University of Denmark, Department of Chemical Engineering
ISBN (Print): 87-90142-10-1
Original language: English
Main Research Area: Technical/natural sciences
Electronic versions: Jo_o_Coutinho.pdf
Publication: Research › Ph.D. thesis – Annual report year: 1995
Understanding Miscibility in Gas Injection Processes

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering
Authors: Stenby, E. H. (Intern)
Number of pages: 548
Publication date: 1994
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 41426
Publication: Research › Poster – Annual report year: 1994

Projects:

High Pressure Phase Behavior of Asymmetric Mixtures for Oil Production
Department of Chemistry
Period: 01/02/2017 → 31/01/2020
Number of participants: 4
Phd Student:
Liu, Yiqun (Intern)
Supervisor:
Regueira Muñiz, Teresa (Intern)
Stenby, Erling Halfdan (Intern)
Main Supervisor:
Yan, Wei (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Privatist
Project: PhD

Estimation of Matrix Flow contribution in naturally fractured reservoirs
Department of Chemical and Biochemical Engineering
Period: 01/09/2015 → 31/08/2018
Number of participants: 4
Phd Student:
Brand Ferrell, Justin (Intern)
Supervisor:
Stenby, Erling Halfdan (Intern)
Yan, Wei (Intern)
Main Supervisor:
Shapiro, Alexander (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Privatist
Project: PhD

Computation of Simultaneous Phase and Chemical Equilibrium
Department of Chemistry
Period: 15/12/2014 → 15/01/2018
Number of participants: 3
Phd Student:
Tsanas, Christos (Ekstern)
Compositional Simulation of Heavy Oil Production with Steam and Solvent

Department of Chemistry
Period: 01/09/2014 → 13/12/2017
Number of participants: 7
PhD Student:
Paterson, Duncan (Intern)
Supervisor:
Michelsen, Michael Locht (Intern)
Stenby, Erling Halfdan (Intern)
Main Supervisor:
Yan, Wei (Intern)
Examiner:
Henriksen, Niels Engholm (Intern)
Hendriks, Eric Maria (Ekstern)
Montel, François (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)
Project: PhD

Compositional Reservoir Simulation Involving Complex Pase Equilibria

Department of Chemistry
Period: 01/07/2014 → 30/09/2017
Number of participants: 7
PhD Student:
Sandoval Lemus, Diego Rolando (Intern)
Supervisor:
Michelsen, Michael Locht (Intern)
Stenby, Erling Halfdan (Intern)
Main Supervisor:
Yan, Wei (Intern)
Examiner:
Shapiro, Alexander (Intern)
Galliéro, Guillaume (Ekstern)
Koch, Oliver (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Eksternt finansieret virksomhed
Project: PhD

Relations
Publications:
Phase Equilibrium Modeling for Shale Production Simulation
Project: PhD

PhD Scholarship in Nanoscale Imaging of the Aqueous Processes of Precipitation, Dispersion and Imbition

Department of Micro- and Nanotechnology
Period: 15/05/2014 → 13/09/2017
Number of participants: 7
Phd Student:
Laganà, Simone (Intern)
Supervisor:
Burrows, Andrew (Intern)
Stenby, Erling Halfdan (Intern)
Main Supervisor:
Mølhave, Kristian (Intern)
Examiner:
Booth, Tim (Intern)
Davis, Zachary James (Intern)
Xu, Qiang (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Samfinansieret - Andet
Project: PhD

Study of High Pressure and High Temperature Reservoir Fluids
Department of Chemistry
Period: 15/12/2013 → 25/08/2017
Number of participants: 6
Phd Student:
Varzandeh, Farhad (Intern)
Supervisor:
Stenby, Erling Halfdan (Intern)
Main Supervisor:
Yan, Wei (Intern)
Examiner:
Møller, Klaus Braagaard (Intern)
Lindeloff, Niels (Intern)
Montel, François (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Eksternt finansieret virksomhed

Relations
Publications:
Modeling Study of High Pressure and High Temperature Reservoir Fluids
Project: PhD

Measurement and modelling of phase equilibrium of oil-water polar chemicals
Department of Chemical and Biochemical Engineering
Period: 01/06/2011 → 11/03/2015
Number of participants: 7
Phd Student:
Frost, Michael Grynnerup (Intern)
Supervisor:
Stenby, Erling Halfdan (Intern)
von Solms, Nicolas (Intern)
Main Supervisor:
Kontogeorgis, Georgios (Intern)
Examiner:
Yan, Wei (Intern)
Hendriks, Eric Maria (Ekstern)
Knudsen, Kim (Intern)
Financing sources
Source: Internal funding (public)
Name of research programme: Eksternt finansieret virksomhed
Project: PhD

Smart Water
Water flooding is a standard method to extract extra oil from mature fields. International research suggests that the impact may be increased by modifying salinity or other features of the injected water. Involving industrial partners the Smart Water project led by CERE is focussed on both theoretical understanding and practical applications.

Funded by Energistyrelsen, DONG Energy and Maersk Oil
Center for Energy Resources Engineering
Department of Chemistry
Department of Civil Engineering
Section for Geotechnics and Geology
Period: 01/06/2011 → 30/09/2014
Number of participants: 2
Project ID: 50845
Project Manager, academic: Stenby, Erling Halfdan (Intern)
Project Coordinator: Fabricius, Ida Lykke (Intern)

BioRec
BioRec is a Danish research program involving several industrial and research partners. The program is focussed on both Microbial Enhanced Oil Recovery (MEOR) and enzymatic enhanced oil recovery while also looking into innovative use of biotechnology in relation to prevention of corrosion and gas hydrate formation. The program is led by CERE.

Funded by HTF
Center for Energy Resources Engineering
Department of Chemistry
Period: 15/03/2011 → 30/09/2015
Number of participants: 1
Project Manager, academic: Stenby, Erling Halfdan (Intern)

Disc. Meeting, løbende
Funded by: Deltagerbetaling
Center for Energy Resources Engineering
Department of Chemistry
Period: 01/02/2011 → 31/12/2020
Number of participants: 1
Project ID: 50807
Project Manager, academic: Stenby, Erling Halfdan (Intern)

Integrated Modeling of Oil Reservoirs - history matching and geostatistical analysis
National Space Institute
Period: 15/06/2010 → 14/05/2014
Number of participants: 7
Phd Student: Melnikova, Yulia (Intern)
Supervisor:
Shapiro, Alexander (Intern)
Stenby, Erling Halfdan (Intern)
Main Supervisor:
Mosegaard, Klaus (Intern)
Examiner:
Finlay, Chris (Intern)
Demyanov, Vasily V. (Ekstern)
Khan, Amir (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

Integrated Modeling of Oil Reservoirs - seismic and geostatistical analysis
Department of Informatics and Mathematical Modeling
Period: 01/03/2010 → 30/08/2013
Number of participants: 6
Phd Student:
Lange, Katrine (Intern)
Supervisor:
Hansen, Per Christian (Intern)
Stenby, Erling Halfdan (Intern)
Main Supervisor:
Mosegaard, Klaus (Intern)
Examiner:
Knudsen, Per (Intern)
Kolbjørnsen, Odd (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

CERE Administration
Center for Energy Resources Engineering
Department of Chemistry
Period: 01/01/2010 → 10/10/2020
Number of participants: 1
Project ID: 50678
Project participant:
Stenby, Erling Halfdan (Intern)
Project

Stochastic Modelling Polydisperse Transport of Particles in Porous Media
Department of Chemical and Biochemical Engineering
Period: 01/10/2009 → 17/12/2012
Number of participants: 6
Phd Student:
Yuan, Hao (Intern)
Supervisor:
Stenby, Erling Halfdan (Intern)
Main Supervisor:
Shapiro, Alexander (Intern)
Examiner:
Szabo, Peter (Ekstern)
Bradford, Scott Alan (Ekstern)
Lindeloff, Niels (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

Thermodynamic Modelling of Acid Gases - Alkanolamine Systems
Department of Chemical and Biochemical Engineering
Period: 01/04/2009 → 21/05/2013
Number of participants: 6
Phd Student:
Sadegh, Negar (Intern)
Supervisor:
Stenby, Erling Halfdan (Intern)
Main Supervisor:
Thomsen, Kaj (Intern)
Examiner:
Kontogeorgis, Georgios (Intern)
Knudsen, Kim (Intern)
Koch, Oliver (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Eksternt finansieret virksomhed
Project: PhD

Ionic Liquids for CO2 Capture
Funded by FIST, DONG Energy and Mærsk Oil
DOC 09/00224
Under lukning
Center for Energy Resources Engineering
Department of Chemistry
Period: 01/03/2009 → 01/06/2011
Number of participants: 1
Acronym: Ionic Liquids
Project ID: 50644
Project participant:
Stenby, Erling Halfdan (Intern)

Advanced Waterflooding in Low Permeable Carbonate Reservoirs
Department of Chemical and Biochemical Engineering
Period: 01/01/2009 → 27/06/2012
Number of participants: 7
Phd Student:
Zahid, Adeel (Intern)
Supervisor:
Stenby, Erling Halfdan (Intern)
Yan, Wei (Intern)
Main Supervisor:
Shapiro, Alexander (Intern)
Examiner:
Thomsen, Kaj (Intern)
Christensen, Helle Foged (Intern)
Spildo, Kristine (Ekstern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: Eksternt finansieret virksomhed
Project: PhD

**Reactive Transport in Oil Recovery Processes**
Department of Chemical and Biochemical Engineering
Period: 01/01/2009 → 31/05/2011
Number of participants: 4
Phd Student:
Jain, Priyanka (Intern)
Supervisor:
Stenby, Erling Halfdan (Intern)
von Solms, Nicolas (Intern)
Main Supervisor:
Shapiro, Alexander (Intern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

**CO₂ capture from flue gas using amino acid salt solutions**
Department of Chemical and Biochemical Engineering
Period: 01/12/2008 → 21/11/2012
Number of participants: 6
Phd Student:
Lerche, Benedicte Mai (Intern)
Supervisor:
Stenby, Erling Halfdan (Intern)
Main Supervisor:
Thomsen, Kaj (Intern)
Examiner:
von Solms, Nicolas (Intern)
Jens, Klaus-Joachim (Ekstern)
Jensen, Jørgen Peter (Intern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: Eksternt finansieret virksomhed
Project: PhD

**CompSim**
DOC 08/00420
prolonged until 30. april 2012
Center for Energy Resources Engineering
Department of Chemistry
Period: 10/11/2008 → 09/11/2010
Number of participants: 1
Project ID: 50588
Project participant:
Stenby, Erling Halfdan (Intern)
Project
Multiphase flows in porous media
Department of Chemical and Biochemical Engineering
Period: 01/09/2008 → 14/12/2011
Number of participants: 5
Phd Student: Zhang, Xuan (Intern)
Supervisor: Stenby, Erling Halfdan (Intern)
Main Supervisor: Shapiro, Alexander (Intern)
Examiner: Yan, Wei (Intern)
Øbro, Hans (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

Enhanced Oil Recovery with Surfactant Flooding
Department of Chemical and Biochemical Engineering
Period: 01/05/2008 → 27/06/2012
Number of participants: 6
Phd Student: Sandersen, Sara Bülow (Intern)
Supervisor: Stenby, Erling Halfdan (Intern)
Main Supervisor: von Solms, Nicolas (Intern)
Examiner: Yan, Wei (Intern)
Skauge, Arne (Ekstern)
Sparsø, Flemming Vang (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU) Samf.
Project: PhD

Distribution of Complex Chemicals in Oil-Water Systems
Department of Chemical and Biochemical Engineering
Period: 01/04/2008 → 08/02/2012
Number of participants: 7
Phd Student: Riaz, Muhammad (Intern)
Supervisor: Stenby, Erling Halfdan (Intern)
Yan, Wei (Intern)
Main Supervisor: Kontogeorgis, Georgios (Intern)
Examiner: von Solms, Nicolas (Intern)
Hemptinne, Jean-Charles de (Ekstern)
Knudsen, Kim (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Eksternt finansieret virksomhed
CO2 Capture with Aqueous Ammonia

Department of Chemical and Biochemical Engineering
Period: 01/02/2008 → 14/12/2011
Number of participants: 7
Phd Student:
Darde, Victor Camille Alfred (Intern)
Supervisor:
Stenby, Erling Halfdan (Intern)
von Well, Willy J. M. (Ekstern)
Main Supervisor:
Thomsen, Kaj (Intern)
Examiner:
von Solms, Nicolas (Intern)
Kotdawala, Rasesh R. (Ekstern)
Svendsen, Hallvard Fjøsne (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: ErhvervsPhD-ordningen VTU
Project: PhD

Oliespild i Arktis

Department of Civil Engineering
Period: 01/11/2007 → 08/12/2010
Number of participants: 7
Phd Student:
Fritt-Rasmussen, Janne (Intern)
Supervisor:
Brandvik, Per Johan (Ekstern)
Stenby, Erling Halfdan (Intern)
Main Supervisor:
Villumsen, Ame (Intern)
Examiner:
von Solms, Nicolas (Intern)
Collin-Hansen, Chr. (Ekstern)
Lykke-Andersen, Holger (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Offentlig finansiering
Project: PhD

ADORE - Advanced Oil Recovery Methods
As easily accessible oil reserves are becoming scarcer, the need for new approaches in Enhanced Oil Recovery (EOR) is growing. The Advanced Oil Recovery Methods (ADORE) project led by CERE encompasses a range of research disciplines with the objective of adding to recoverable hydrocarbon reserves via novel or improved EOR methodologies.

Funded by FIST

Center for Energy Resources Engineering

Department of Chemistry
Period: 01/09/2007 → 01/01/2013
Number of participants: 1
Acronym: ADORE
Project ID: 50548
Project Manager, academic:
Design of CO2 Capture Units using Aqueous Alkanolamines
Department of Chemical and Biochemical Engineering
Period: 15/02/2007 → 01/09/2010
Number of participants: 7
Phd Student:
Faramarzi, Leila (Intern)
Supervisor:
Stenby, Erling Halfdan (Intern)
Thomsen, Kaj (Intern)
Main Supervisor:
Kontogeorgis, Georgios (Intern)
Examiner:
Shapiro, Alexander (Intern)
Behrens, Paul K. (Ekstern)
von Well, Willy J. M. (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

Øget olieudvinding gennem CO2 udnyttelse
Center for Energy Resources Engineering
Department of Chemistry
Period: 01/01/2007 → 31/12/2009
Number of participants: 1
Project ID: 50505
Project Manager, academic:
Stenby, Erling Halfdan (Intern)

Co2 Injection in Low Permeable Oil and Gas Reservoir
Department of Chemical and Biochemical Engineering
Period: 15/09/2006 → 21/12/2010
Number of participants: 6
Phd Student:
Niu, Ben (Intern)
Supervisor:
Stenby, Erling Halfdan (Intern)
Yan, Wei (Intern)
Main Supervisor:
Shapiro, Alexander (Intern)
Examiner:
von Solms, Nicolas (Intern)
Skauge, Arne (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: DTU-lønnet stipendie
Project: PhD

Avanceret Reservoir Simulering
Department of Chemical and Biochemical Engineering
Period: 01/09/2006 → 24/11/2010
Number of participants: 7
Phd Student:
Nielsen, Sidsel Marie (Intern)
Supervisor:
Michelsen, Michael Locht (Intern)
Stenby, Erling Halfdan (Intern)
Main Supervisor:
Shapiro, Alexander (Intern)
Examiner:
Mosegaard, Klaus (Intern)
Aavatsmark, Ivar (Ekstern)
Jørgensen, Marianne (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: 1/3 DTU-stip, 2/3 FUR/andet
Project: PhD

Sponsors til IVC-SEP
Center for Energy Resources Engineering
Department of Chemistry
Period: 01/09/2006 → 10/10/2020
Number of participants: 1
Project ID: 50767
Project Manager, academic:
Stenby, Erling Halfdan (Intern)
Project

Modelling of CO2 Capture
Funded by FIST, DONG Energy and Mærsk Oil
Under lukning
Center for Energy Resources Engineering
Department of Chemistry
Period: 01/05/2006 → 01/07/2010
Number of participants: 1
Project ID: 50421
Project Manager, academic:
Stenby, Erling Halfdan (Intern)
Project

Development of Derivatized Hyaluronic Acid and Formulation of Nanocapsules for Delivery of Cosmetic Actives and Pharmaceutical Drugs
Department of Chemical and Biochemical Engineering
Period: 15/05/2005 → 03/11/2008
Number of participants: 9
Phd Student:
Eenschooten, Corinne Diane (Intern)
Supervisor:
Gurny, Robert (Ekstern)
Guillaumie, Fanny (Intern)
Schwach-Abdellaoui, Khadija (Ekstern)
Stenby, Erling Halfdan (Intern)
Main Supervisor:
Kontogeorgis, Georgios (Intern)
Petrochallenge – a Competition for High Schools
By combining fun and education, the international PetroChallenge competition encourages high school students in a growing number of countries to take interest in energy resources engineering. CERE has been organizing the national branch of the annual competition since its introduction in Denmark in 2005.

Funded by DONG Energy and Maersk Oil

History Matcging using Stochastic Methods
Department of Chemical and Biochemical Engineering
Period: 01/09/2004 → 15/05/2008
Number of participants: 6
Phd Student:
Johansen, Kent (Ekstern)
Supervisor:
Stenby, Erling Halfdan (Intern)
Main Supervisor:
Shapiro, Alexander (Intern)
Examiner:
Michelsen, Michael Locht (Intern)
Hu, Lin Y. (Ekstern)
Mosegaard, Klaus (Intern)

Avanceret Reservoirsimulering
Department of Chemical and Biochemical Engineering
Period: 15/08/2004 → 16/05/2008
Number of participants: 7
Phd Student:
Kristensen, Morten Rode (Intern)
Supervisor:
Michelsen, Michael Locht (Intern)
Thomsen, Per Grove (Intern)
Main Supervisor:
Stenby, Erling Halfdan (Intern)
Examiner:
Shapiro, Alexander (Intern)
Aavatsmark, Ivar (Ekstern)
Saaf, Fredrik (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: DTU-lønnet stipendie
Project: PhD

Temperaturafhængighed af bjergartsmekaniske egenskaber
Department of Civil Engineering
Period: 01/08/2004 → 01/06/2011
Number of participants: 7
Phd Student:
Andreassen, Katrine Alling (Intern)
Supervisor:
Hededal, Ole (Intern)
Krogsbøll, Anette (Intern)
Main Supervisor:
Foged, Niels Nielsen (Intern)
Examiner:
Stenby, Erling Halfdan (Intern)
Holt, Rune M. (Ekstern)
Schroeder, Christian (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: DTU-lønnet stipendie
Project: PhD

Corrosion in Wet Gas Pipelines
Department of Chemical and Biochemical Engineering
Period: 01/02/2004 → 25/03/2008
Number of participants: 6
Phd Student:
Fosbøl, Philip Loldrup (Intern)
Supervisor:
Stenby, Erling Halfdan (Intern)
Main Supervisor:
Thomsen, Kaj (Intern)
Examiner:
Mollerup, Jørgen (Intern)
Dugstad, Arne (Ekstern)
Rislund, Ebbe (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: DTU, Samfinansiering
Project: PhD

Modelling of Enzymatic Hydrolysis of Lignocellulosic Material
Department of Systems Biology
Period: 01/01/2004 → 26/10/2007
Number of participants: 8
Phd Student:
Andersen, Natalija (Intern)
Supervisor:
Johansen, Katja Salomon (Ekstern)
Michelsen, Michael Locht (Intern)
Stenby, Erling Halfdan (Intern)
Main Supervisor:
Olsson, Lisbeth (Intern)
Examiner:
Gernaey, Krist V. (Intern)
Felby, Claus (Ekstern)
Tjerneld, Folke (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: DTU, Samfinansiering
Project: PhD

CO2 Capture from Coal Fired Power Plants

Department of Chemical and Biochemical Engineering
Period: 01/11/2003 → 16/02/2007
Number of participants: 7
Phd Student:
Gabrielsen, Jostein (Intern)
Supervisor:
Kontogeorgis, Georgios (Intern)
Michelsen, Michael Locht (Intern)
Main Supervisor:
Stenby, Erling Halfdan (Intern)
Examiner:
von Solms, Nicolas (Intern)
Fogh, Folmer (Ekstern)
Solbraa, Even (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Offentlig finansiering
Project: PhD

Modelling of Complex Mixtures Containing Hydrogen Bonding Molecules using CPA EOS

Department of Chemical and Biochemical Engineering
Period: 01/11/2003 → 22/01/2007
Number of participants: 7
Phd Student:
Folas, Georgios (Intern)
Supervisor:
Michelsen, Michael Locht (Intern)
Stenby, Erling Halfdan (Intern)
Main Supervisor:
Kontogeorgis, Georgios (Intern)
Examiner:
Abildskov, Jens (Intern)
Economou, Ioannis (Intern)
Knudsen, Kim (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Eksternt finansieret virksomhed
Project: PhD
Experimental Studies and Modeling of Asphaltene Precipitation Caused by Gas Injection

Department of Chemical and Biochemical Engineering
Period: 01/05/2003 → 01/09/2006
Number of participants: 6
Phd Student:
Verdier, Sylvain Charles Roland (Intern)
Supervisor:
Ivar Andersen, Simon (Intern)
Main Supervisor:
Stenby, Erling Halfdan (Intern)
Examiner:
Kontogeorgis, Georgios (Intern)
Lindeloff, Niels (Intern)
Randzio, Stanislaw L. (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut/centerfinansieret
Project: PhD

Modelling of Mineral Scale Deposition

Department of Chemical and Biochemical Engineering
Period: 01/10/2002 → 22/12/2005
Number of participants: 5
Phd Student:
Villafafila Garcia, Ada (Intern)
Supervisor:
Stenby, Erling Halfdan (Intern)
Main Supervisor:
Thomsen, Kaj (Intern)
Examiner:
Jensen, Jørgen Peter (Intern)
Kleinitz, Wolfram (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut/centerfinansieret
Project: PhD

Compositional Streamline Simulation.

Department of Chemical and Biochemical Engineering
Period: 01/09/2001 → 28/01/2005
Number of participants: 7
Phd Student:
Berenblyum, Roman (Ekstern)
Supervisor:
Michelsen, Michael Locht (Intern)
Shapiro, Alexander (Intern)
Main Supervisor:
Stenby, Erling Halfdan (Intern)
Examiner:
Foged, Niels Tækker (Intern)
Bedrikovetsky, Pavel (Ekstern)
Jakupsstovu, Sigurd (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Anden sektorministeriel finans
**Transport Coefficients in Hydrocarbon Mixtures under Microgravity Conditions**

Department of Chemical and Biochemical Engineering  
Period: 01/08/2001 → 18/03/2005  
Number of participants: 6  
Phd Student: Gonzales Bagnoli, Mariana G. (Intern)  
Supervisor: Stenby, Erling Halfdan (Intern)  
Main Supervisor: Shapiro, Alexander (Intern)  
Examiner: Mollerup, Jørgen (Intern)  
Knudsen, Kim (Intern)  
Montel, François (Ekstern)  

**Financing sources**  
Source: Internal funding (public)  
Name of research programme: Forskningsrådsstipendium  
Project: PhD

**Mætningsfordeling og petrofysiske egenskaber i lav-permable Nordø kalkreservoirer**

Department of Chemical and Biochemical Engineering  
Period: 16/11/2000 → 09/12/2005  
Number of participants: 2  
Phd Student: Nielsen, Carsten Møller (Intern)  
Main Supervisor: Stenby, Erling Halfdan (Intern)  

**Financing sources**  
Source: Internal funding (public)  
Name of research programme: Forskerakademiets Samfinansier  
Project: PhD

**Dissolution and Adsorption of Light Hydrocarbons in Drilling Muds, Prediction of the Nature of a REsevoir Fluid Based on Gas Shows**

Department of Chemical and Biochemical Engineering  
Period: 01/10/2000 → 14/07/2006  
Number of participants: 6  
Phd Student: Liege, Xavier Christophe (Intern)  
Supervisor: Shapiro, Alexander (Intern)  
Main Supervisor: Stenby, Erling Halfdan (Intern)  
Examiner: Fabricius, Ida Lykke (Intern)  
Marnat, Serge (Ekstern)  
Øbro, Hans (Ekstern)  

**Financing sources**  
Source: Internal funding (public)  
Name of research programme: Samarbejdsaftalefinans  
Project: PhD
Phase behavior and transport processes in porous media
Department of Chemical and Biochemical Engineering
Period: 01/04/2000 → 28/02/2001
Number of participants: 2
Phd Student:
Madsen, Jesper (Intern)
Main Supervisor:
Stenby, Erling Halfdan (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Offentlig finansiering
Project: PhD

Phase behavior of Aqueous of Surfactant Solution
Department of Chemical and Biochemical Engineering
Period: 01/01/2000 → 26/02/2004
Number of participants: 6
Phd Student:
Cheng, Hongyuan (Intern)
Supervisor:
Kontogeorgis, Georgios (Intern)
Main Supervisor:
Stenby, Erling Halfdan (Intern)
Examiner:
Ivar Andersen, Simon (Intern)
Birdi, Kulbir S. (Ekstern)
Maurer, Gerd (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Centerfinansieret
Project: PhD

Fasefordeling af produktionskemikalier
Department of Chemical and Biochemical Engineering
Period: 01/05/1999 → 21/02/2003
Number of participants: 6
Phd Student:
Derawi, Samer (Intern)
Supervisor:
Kontogeorgis, Georgios (Intern)
Main Supervisor:
Stenby, Erling Halfdan (Intern)
Examiner:
Ivar Andersen, Simon (Intern)
Economou, Ioannis (Intern)
Knudsen, Kim (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Ansat eksternt CAMP
Project: PhD

Kompositionel reservoisimuselring af gas injektionsprocesser
Department of Chemical and Biochemical Engineering
Period: 01/08/1998 → 28/02/2003
Number of participants: 5
Phd Student: Jakupsstovu, Sigurd (Intern)
Main Supervisor: Stenby, Erling Halfdan (Intern)
Examiner: Shapiro, Alexander (Intern)
Jansson, John (Ekstern)
Olsen, Henrik (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Kandidatstipendium ansat på DT
Project: PhD

Kulbrinters egenskaber ved høje tryk og temperaturer
Department of Chemical and Biochemical Engineering
Number of participants: 5
Phd Student: Zeberg-Mikkelsen, Claus Kjær (Intern)
Main Supervisor: Stenby, Erling Halfdan (Intern)
Examiner: Fernández, Josefa (Ekstern)
Knudsen, Kim (Intern)
Thomsen, Kaj (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Eksternt EU-finansieret
Project: PhD

Modellering af kulbrinteblandingers faseopførsel ved høje tryk og temperaturer
Department of Chemical and Biochemical Engineering
Number of participants: 5
Phd Student: Halldórsson, Snorri (Intern)
Main Supervisor: Stenby, Erling Halfdan (Intern)
Examiner: Michelsen, Michael Locht (Intern)
Hendriks, Eric M. (Ekstern)
Knudsen, Kim (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: DTU-lønnet stipendie
Project: PhD

Measurement of Phase Equilibria and Transport Properties (C.2)
PVT studies on petroleum reservoir fluids in the fibre optic mini PVT cell and the Mercury free ROP set-up. True boiling point (TBP) distillation of dead crude oils and gas condensates. Assessment of purity of TBP fractions by gas chromatographic (GC) analysis. Measurement of the viscosity of TBP cuts, dead crude oils, and gas condensates using the Anton-Paar microviscometer.

Department of Chemical and Biochemical Engineering
Modelling of Phase Equilibria and Transport Properties (C.1)
Modelling of the phase behavior of reservoir fluids within a porous medium and during injection of gases.

Department of Chemical and Biochemical Engineering
Period: 01/01/1998 → 31/12/1998
Number of participants: 5

Project participant:
Michelsen, Michael Locht (Intern)
Shapiro, Alexander (Intern)
Dandekar, Abhijit (Intern)
Jessen, Kristian (Intern)

Project Manager, organisational:
Stenby, Erling Halfdan (Intern)

Phase Behavior of Asphaltene Containing Reservoir Fluids (C.5)
Developed procedures for correlation and prediction of the onset of asphaltene precipitation.

Department of Chemical and Biochemical Engineering
Period: 01/01/1998 → 31/12/1998
Number of participants: 5

Project participant:
Pedersen, Carsten (Intern)
Dang, Tran Thuong (Intern)
Lindeloff, Niels (Intern)

Project Manager, organisational:
Stenby, Erling Halfdan (Intern)

Phase Equilibria Including an Aqueous Phase (C.3)
Prediction of phase equilibria of brine - oil systems containing production chemicals. An investigation of the relation to the octanol - water partition coefficient.

Department of Chemical and Biochemical Engineering
Period: 01/01/1998 → 31/12/1998
Number of participants: 1

Project Manager, organisational:
Stenby, Erling Halfdan (Intern)

Recovery processes (C.7)
Experimental and theoretical investigations of oil recovery processes with emphasis on low permeable reservoir rocks.

Department of Chemical and Biochemical Engineering
Period: 01/01/1998 → 31/12/1998
Number of participants: 8

Project participant:
Mogensen, Kristian (Intern)
Poulsen, Søren (Intern)
Simulation of IOR/EOR with advanced thermodynamic models (C.8)

Department of Chemical and Biochemical Engineering
Period: 01/01/1998 → 31/12/1998
Number of participants: 3
Project participant:
Jørgensen, Marianne (Intern)
Christensen, Jes Reimer (Intern)

Project Manager, organisational:
Stenby, Erling Halfdan (Intern)

Wax Formation in Reservoir Fluids (C.6)
To measure high pressure solid phase transitions using real fluids and model systems.

Department of Chemical and Biochemical Engineering
Period: 01/01/1998 → 31/12/1998
Number of participants: 3
Project participant:
Ivar Andersen, Simon (Intern)
Lindeloff, Niels (Intern)

Project Manager, organisational:
Stenby, Erling Halfdan (Intern)

Effekt af varmebehandling på begkvalitet

Department of Chemical and Biochemical Engineering
Period: 01/12/1997 → …
Number of participants: 6
Phd Student:
Ascanius, Birgit Elkjær (Intern)
Supervisor:
Stenby, Erling Halfdan (Intern)
Main Supervisor:
Ivar Andersen, Simon (Intern)
Examiner:
Østergaard, Knud (Intern)
Stokke, Per (Ekstern)
Øye, Harald A. (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Erhvervsforskerordningen
Project: PhD

Kolloide egenskaber af asfaltener i oljer

Department of Chemical and Biochemical Engineering
Oil recovery processes
Department of Chemical and Biochemical Engineering
Period: 01/08/1997 → 14/09/2001
Number of participants: 5
Phd Student:
Poulsen, Susanne (Intern)
Main Supervisor:
Stenby, Erling Halfdan (Intern)
Examiner:
Foged, Niels Tækker (Intern)
Patzek, Tadeusz W. (Ekstern)
Reffstrup, Jan Otto (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Center-Finansieret-SU
Project: PhD

Raman Spectroscopy Analysis of Phase Equilibria
Phase Equilibria in multicomponent systems, e.g. in fuels, oil and gasses, are studied by Raman and IR spectroscopy. The project is a ph.d. project for Susanne Brunsgaard Hansen, supported by The National Oil and Gas Company of Denmark, The Nordic Energy Research Program and The Danish Technical Research Council.

Department of Chemistry
Department of Chemical and Biochemical Engineering
Center for Energy Resources Engineering
DONG Energy A/S
Nordiske Energiforskningsprogram
Period: 01/07/1997 → 30/01/2001
Number of participants: 3
Project participant:
Hansen, Susanne Brunsgaard (Intern)
Stenby, Erling Halfdan (Intern)
Project Manager, organisational:
Berg, Rolf W. (Intern)

Financing sources
Source: Unknown
Name of research programme: Ukendt
Amount: 648,000.00 Danish Kroner
Gasinjektion i
department of Chemical and Biochemical Engineering
Period: 01/02/1997 → 31/07/2000
Number of participants: 4
PhD Student: Jessen, Kristian (Intern)
Supervisor: Michelsen, Michael Locht (Intern)
Main Supervisor: Stenby, Erling Halfdan (Intern)
Examiner: Villadsen, John (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: DTU-Su Stipendium, Eksperiment
Project: PhD

Dannelse af organiske faste faser i kulbrinteblandinger
department of Chemical and Biochemical Engineering
Period: 01/02/1996 → ...
Number of participants: 2
PhD Student: Lindeloff, Niels (Intern)
Main Supervisor: Stenby, Erling Halfdan (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Blandet Finansiering-SU
Project: PhD

Termodynamik i kompositionel reservoir simulering
department of Chemical and Biochemical Engineering
Period: 01/08/1995 → ...
Number of participants: 3
PhD Student: Christensen, Jes Reimer (Intern)
Main Supervisor: Stenby, Erling Halfdan (Intern)
Examiner: Frørup, Mikael Dan (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Blandet Finansiering-SU
Project: PhD
Forædling af rapsolie
Department of Systems Biology
Period: 01/02/1995 → …
Number of participants: 4
Phd Student:
Balchen, Steen (Intern)
Main Supervisor:
Adler-Nissen, Jens (Intern)
Examiner:
Nordstrøm, Leif (Ekstern)
Stenby, Erling Halfdan (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Erhvervsforskerordningen
Project: PhD

Fortrængningsprocesser i Porøse Medier
Department of Chemical and Biochemical Engineering
Period: 01/02/1995 → 15/07/1998
Number of participants: 2
Phd Student:
Mogensen, Kristian (Intern)
Main Supervisor:
Stenby, Erling Halfdan (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsstip.-SU, Eksp
Project: PhD

Modellering af reservoirfluider ved højt tryk og høj temperatur
Department of Chemical and Biochemical Engineering
Period: 01/08/1994 → 22/03/2000
Number of participants: 2
Phd Student:
Gommesen, Søren (Intern)
Main Supervisor:
Stenby, Erling Halfdan (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Ef-Finansieret, Stipen.-SU
Project: PhD

Development of an improved microwave apparatus for detection of high pressure dew and bubble points
Department of Chemical and Biochemical Engineering
Period: 09/12/1992 → 27/02/1997
Number of participants: 2
Phd Student:
Sendrup, Peter William (Intern)
Main Supervisor:
Stenby, Erling Halfdan (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Gammel ordning u/skema-SU
**Mikroskala modelling og eksperimentelle studier af strømning i porøse medier**

Technical University of Denmark  
**Period:** 09/12/1992 → 01/07/1996  
**Number of participants:** 2  
**PhD Student:** Sendrup, Linda (Intern)  
**Main Supervisor:** Stenby, Erling Halfdan (Intern)

**Financing sources**  
Source: Internal funding (public)  
Name of research programme: Gammel ordning u/skema-SU  
**Project:** PhD

**Phase behavior of near critical hydrocarbon fluids**

Technical University of Denmark  
**Period:** 09/12/1992 → 01/07/1996  
**Number of participants:** 2  
**PhD Student:** Dønkjær, Tina (Intern)  
**Main Supervisor:** Stenby, Erling Halfdan (Intern)

**Financing sources**  
Source: Internal funding (public)  
Name of research programme: Gammel ordning u/skema-SU  
**Project:** PhD

**Phase Equilibria in petroleum fluids: multiphase regions and waxformation.**

Department of Chemical and Biochemical Engineering  
**Period:** 01/12/1992 → 23/04/1996  
**Number of participants:** 2  
**PhD Student:** Coutinho, Joao (Intern)  
**Main Supervisor:** Stenby, Erling Halfdan (Intern)

**Financing sources**  
Source: Internal funding (public)  
Name of research programme: anden international finansieri  
**Project:** PhD

**Simulering af forbedret olieindvinding (IOR) med avancerede termodynamiske modeller**

Department of Chemical and Biochemical Engineering  
**Period:** 01/11/1992 → 27/02/1997  
**Number of participants:** 2  
**PhD Student:** Jørgensen, Marianne (Intern)  
**Main Supervisor:** Stenby, Erling Halfdan (Intern)

**Financing sources**  
Source: Internal funding (public)  
Name of research programme: Nordisk finansiering  
**Project:** PhD
Termodynamiske modeller i kompositionel reservoir-simulering

Department of Chemical and Biochemical Engineering
Period: 01/05/1991 → 16/02/1994
Number of participants: 2
Phd Student:
Peng, Wang (Intern)
Main Supervisor:
Stenby, Erling Halfdan (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Gammel ordning u/skema-SU
Project: PhD

Studies of the phase behavior and physical properties of hydrocarbon fluids

Department of Chemical and Biochemical Engineering
Period: 01/01/1991 → 21/03/1994
Number of participants: 2
Phd Student:
Amin, Robert (Intern)
Main Supervisor:
Stenby, Erling Halfdan (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Selvfinansierende (privatist)
Project: PhD

Activities:

Thermodynamic modeling of sour gas cleaning process with alkanolamine: Oral presentation at the 25th European SYmposium on Applied Thermodynamics (ESAT), St.Petersburg, Russia
Period: 1 Jan 2011 → …
Erling Halfdan Stenby (Speaker)
Department of Chemistry
Center for Energy Resources Engineering

Related external organisation

Unknown external organisation
Activity: Talks and presentations › Conference presentations

Thermodynamic modeling of sour gas cleaning process with alkanolamine: Presented at (oral presentation) CERE discussion meeting, Hillerød
Period: 1 Jan 2011 → …
Erling Halfdan Stenby (Speaker)
Department of Chemistry
Center for Energy Resources Engineering

Related external organisation

Unknown external organisation
Activity: Talks and presentations › Conference presentations