Influence of Adsorption and Capillary Pressure on Phase Equilibria Inside Shale Reservoirs

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

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Near-wellbore modeling of a horizontal well with Computational Fluid Dynamics

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

Two algorithms are proposed for isothermal multiphase flash. These are referred to as modified RAND and vol-RAND. The former uses the chemical potentials and molar-phase amounts as the iteration variables, while the latter uses chemical potentials and phase volumes to cosolve a pressure-explicit equation of state (EOS) with the equilibrium equations. Compared with the conventional second-order approach using Gibbs-energy minimization, these methods are more structured, with all components in all phases treated in the same way. Both have been derived to include chemical reactions for any number of phases along with the possible simplifications for only phase equilibria. The simple structured implementation of these methods is demonstrated for modified RAND and vol-RAND. The rate of convergence of the methods presented is shown to be the same as the conventional second-order method for isothermal flash. It is demonstrated that the use of an association term [cubic plus association (CPA)] adds little additional computational cost when using vol-RAND compared with a simple cubic Soave-Redlich-Kwong (SRK) without association. The RAND methods scale better in terms of the O(n³) operations as more phases are introduced, and are computationally less expensive than the conventional Gibbs minimization method for more than three phases.

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

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Application of a Crossover Equation of State to Describe Phase Equilibrium and Critical Properties of n-Alkanes and Methane/n-Alkane Mixtures

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

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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.
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.

General information
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.

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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.
Evaluation of equations of state for simultaneous representation of phase equilibrium and critical phenomena

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

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

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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.
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.

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High pressure phase equilibrium of ternary and multicomponent alkane mixtures in the temperature range from (283–473) K

Asymmetric multicomponent alkane mixtures can be used as model systems for reservoir fluids. We have prepared two ternary mixtures, methane/n-butane/n-decane and methane/n-butane/n-dodecane, and two multicomponent mixtures composed of methane/n-butane/n-octane/n-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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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 vmodels 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 vmodels, 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 mostaccurate EoS model for natural gas mixtures. It was found that the non-cubic models are much better than the cubics in density, compressibility, heat capacity and Joule-Thomson coefficient calculation of the well defined light and heavy components in reservoir fluids over a wide temperature and pressure range, GERG-2008 being the best with the lowest deviation among all EoS models. GERG-2008 however gives very large deviations for bubble point pressure calculation of
some heavy and asymmetric binary systems such as n-butane + n-nonane system. This suggests that this EoS and its binary interaction parameters could still be improved for some of the binary pairs. Soave-BWR gives the closest prediction of the thermal properties to that of GERG-2008 among other EoSs tested in this study. The binary VLE calculation showed that PC-SAFT and Soave-BWR are similar to SRK and PR in correlating the important binary pairs in reservoir fluids. Although Soave-BWR and PC-SAFT give smaller average kij values than SRK and PR, they are more sensitive to the change in kij. Phase envelope prediction of synthetic gases showed that all the EoS models were similar for not too asymmetric synthetic gases, with or without the optimal kij values for SRK, PR, PC-SAFT and Soave-BWR. For highly asymmetric synthetic mixtures, Soave-BWR and GERG-2008 tend to predict phase envelopes different from other models where as none of the tested models give satisfactory predictions. For heat capacity and Joule-Thomson coefficients, GERG-2008 and Soave-BWR give the closest predictions. All the evaluated EoS models tend to predict a nearly constant Joule-Thomson coefficient at high pressures. For typical reservoir temperatures, the constant is around -0.5 K/MPa. For non-cubic models like PC-SAFT the characterization method is less mature than the cubic models. A reservoir fluid characterization method for PC-SAFT has been proposed by combining Pedersen's method with a newly developed set of correlations for the PC-SAFT model parameters m, m/ε/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 17 EoS-characterization combinations and 260 reservoir fluids. PC-SAFT with the new general characterization method is shown to give the lowest AAD% and maximum deviation in calculation of saturation pressure, density and STO density, among all the tested characterization methods for PC-SAFT. Application of the new characterization method to SRK and PR improved the saturation pressure calculation in comparison to the original characterization method for SRK and PR. Using volume translation together with the new characterization approach for SRK and PR gives comparable results for density and STO density to that of original characterization for SRK and PR with volume translation. For the PVT database used in this study, cubic EoSs seem to have better performance than PC-SAFT in calculation of saturation pressure; PC-SAFT and cubic models with volume translation show comparable results in calculation of density and STO density. As a preliminary attempt to integrate more analytical information in characterization, we discussed how to modify the existing algorithms to utilize data from both simulated distillation and true boiling point distillation, and in particular, the component distribution information from the simulated distillation. Some analyses have been made on the impact of including more detailed analytical information. Finally, to improve Soave-BWR for mixture calculation, we have tried to develop several new sets of mixing rules for this EoS. The new mixing rules were developed based on some theoretical considerations as well as the previous mixing rules for non-cubic EoS models. In addition, it was tried to create some hybrid mixing rules by combining a new set of mixing rules and the original mixing rules for Soave-BWR. It was shown that some problems with the original Soave-BWR mixing rules can be fixed by the new mixing rules although the overall performance is not significantly improved. Development of mixing rules for non-cubic EoS models is still a semi-empirical process, requiring extensive testing to evaluating their performance. We have developed the code in a structured manner so that the new mixing rules can be quickly tested. It can facilitate further extensive screening of new mixing rules for Soave-BWR or even other non-cubic EoS models.
Phase Equilibrium Modeling for Shale Production Simulation

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

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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 Tammann-Tait correlation of the determined density values. Isobaric thermal expansion coefficients were also calculated based on differentiation from the isobaric fit of density data. We also measured the phase equilibrium of this binary system by using a variable volume cell with full visibility from (293.15-472.47) K for three mixtures with methane mole fractions of 0.4031, 0.6021 and 0.8496. Liquid fraction upon expansion below the saturation pressure has also been determined. Finally different equations of state were used to calculate the experimental density and excess volume data as well as the phase envelope data. No direct regression of the experimental data was involved in most of the calculation in order to provide a fair comparison of the performance of different models.

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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.

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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 cm^3·mol^-1 for the n-hexane + n-decane system and 7.65 cm^3·mol^-1 for the n-hexane + n-hexadecane system. Various equations of state were used to model the measured density data.

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Authors: Regueira , T. (Intern), Yan, W. (Intern), Stenby, E. H. (Intern)
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Modeling the liquid-liquid equilibrium of petroleum fluid and polar compounds containing systems with the PC-SAFT equation of state

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

**General information**

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Organisations: Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering, Department of Chemistry
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- Scopus rating (2013): SJR 1.007 SNIP 1.274 CiteScore 2.31
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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, prediction of multicomponent phase envelopes, and PVT calculation of reservoir fluids. Extensive data are used in the comparison and the four models are treated as equally as possible. We adopt the method of Pedersen et al. as the framework for heptanes plus characterization and the same correlations for estimating the critical properties for SRK, PR and Soave-BWR. For PC-SAFT, new correlations for estimating its model parameters in heptanes plus are developed. The results reveal that the non-cubic models are clearly advantageous in density calculation of pure components. For binary VLE and multicomponent phase envelopes, the results are similar for the four models. For PVT prediction, the non-cubic models show advantages in some high pressure high temperature (HPHT) fluids but no clear advantages in general, indicating the necessity for further improvement of the characterization procedure.
A new approach to model strain change of gelled waxy crude oil under constant stress
Deformation of gelled waxy crude oil with loaded stress is worthy of research for the flow assurance of pipelining system. A dispersion parameter was introduced to characterize the disruption degree of wax crystal structure in crude oil with shear action. Based on fractional calculus theory, a rheological model incorporating dispersion parameter was proposed to describe creep of gelled waxy crude. A discrete and numerical algorithm was proposed to solve the model. Combining with the experimental results of five kinds of waxy crude oil, the model parameters were regressed and found to change monotonously with test temperature. Multiple creep curves of gelled waxy crude oil at a certain temperature can be described with this model.

General information
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Distribution of gas hydrate inhibitor monoethylene glycol in condensate and water systems: Experimental measurement and thermodynamic modeling using the cubic-plus-association equation of state

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

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BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 3.3
Web of Science (2014): Indexed yes
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Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 3.25
ISI indexed (2012): ISI indexed yes
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BFI (2011): BFI-level 2
Scopus rating (2011): CiteScore 3.05
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Web of Science (2011): Indexed yes
Negative Flash for Calculating the Intersecting Key Tie lines in Multicomponent Gas Injection

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

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<td>2017</td>
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ENGINEERING, MINIMUM MISCIBILITY PRESSURE, RACHFORD-RICE, DISPLACEMENTS, EQUILIBRIUM

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

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

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Scopus rating (2016): CiteScore 2.33 SJR 0.869 SNIP 1.155
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BFI (2015): BFI-level 2
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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
On solving the Rachford-Rice equation with higher order methods

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

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BFI (2014): BFI-level 2
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Web of Science (2014): Indexed yes
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Scopus rating (2013): SJR 1.007 SNIP 1.274 CiteScore 2.31
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ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 0.986 SNIP 1.317
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Scopus rating (2009): SJR 1.133 SNIP 1.164
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Scopus rating (2008): SJR 1.227 SNIP 1.09
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Web of Science (2000): Indexed yes
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Rachford-Rice equation, Higher order methods, Flash
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Thermodynamic modeling of complex systems

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

General information
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Scopus rating (2016): CiteScore 3.01 SJR 0.95 SNIP 2.003
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BFI (2015): BFI-level 1
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BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.139 SNIP 1.757 CiteScore 2.3
ISI indexed (2011): ISI indexed yes
Liquid-liquid equilibria data for two binary and two ternary systems are reported in the temperature range of 303.15-323.15 K at atmospheric pressure. The binary systems measured are n-nonane + MEG and ethylbenzene + MEG and the ternary systems are n-nonane + MEG + water and ethylbenzene + MEG + water. These data are satisfactorily correlated (binaries) and predicted (ternaries) using Cubic Plus Association (CPA) equation of state (EoS). CPA is also applied to binary LLE of aromatic hydrocarbon + water and VLE of methane + methanol. Finally the distribution of water and inhibitors (methanol and MEG) in various phases is modeled using CPA. The hydrocarbon phase consists of mixture-1 (methane, ethane, n-butane) or mixture-2 (methane, ethane, propane, n-butane, n-heptane, toluene and n-decane). CPA can satisfactorily predict the water content in the gas phase of the multicomponent systems containing mixture-1 over a range of temperatures and pressures. Similarly the methanol content in the gas phase of mixture-1 + water + methanol systems is predicted satisfactorily with accuracy within experimental uncertainty. For VLLE of mixture-2 + water, mixture-2 + MEG + water and mixture-2 + methanol + water systems, the organic phase compositions are satisfactorily predicted whereas modeling results are relatively less satisfactory for the vapor phase compositions partially due to uncertainties in the experimental data. © 2012 Elsevier B.V.
Online measurement of mass density and viscosity of pL fluid samples with suspended microchannel resonator

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

General information
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Organisations: Department of Micro- and Nanotechnology, Nanoprobes, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Ressources Engineering, Center for Energy Resources Engineering
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Scopus rating (2011): SJR 1.474 SNIP 1.744 CiteScore 4.08
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
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Scopus rating (2010): SJR 1.409 SNIP 1.437
Prediction of the vapor–liquid equilibria and speed of sound in binary systems of 1-alkanols and n-alkanes with the simplified PC-SAFT equation of state

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

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Scopus rating (2016): CiteScore 2.33 SJR 0.869 SNIP 1.155
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Scopus rating (2014): SJR 0.982 SNIP 1.248 CiteScore 2.28
Web of Science (2014): Indexed yes
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BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.152 SNIP 1.286 CiteScore 2.31
ISI indexed (2012): ISI indexed yes
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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
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Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.227 SNIP 1.09
Web of Science (2008): Indexed yes
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Web of Science (2005): Indexed yes
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Speed of sound, PC-SAFT, Vapor–liquid equilibria, 1-Alkanols

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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 Gracia (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.

Approach to Improve Speed of Sound Calculation within PC-SAFT Framework

An extensive comparison of SRK, CPA and PC-SAFT for speed of sound in normal alkanes has been performed. The results reveal that PC-SAFT captures the curvature of speed of sound better than cubic EoS but the accuracy is not satisfactory. Two approaches have been proposed to improve PC-SAFT’s accuracy for speed of sound: (i) putting speed of sound data into parameter estimation; (ii) putting speed of sound data into both universal constants regression and parameter estimation. The results have shown that the second approach can significantly improve the speed of sound (3.2%) prediction while keeping acceptable accuracy for the primary properties, i.e. vapor pressure (2.1%) and liquid density (1.5%). The two approaches have also been applied to methanol, and both give very good results.
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.
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 Ca$^{2+}$ ions with 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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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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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 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 at 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.

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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 Tieline Distance Based Approximation (TDBA) method to get
approximate flash results in the twophase region. The method uses the distance to a previous tieline in the same gridblock to decide whether the approximation should be made. Comparison between the shadow region approach and the approximation approach, including CSAT and TDBA, has been made by using a slitmube 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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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.

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

Today's oil and gas production requires the application of various chemicals in large amounts. To evaluate the effects of those chemicals on the environment, it is of crucial importance to know how much of the chemicals are discharged via produced water and how much is dissolved in the crude oil. The ultimate objective of this work is to develop a predictive thermodynamic model for the mutual solubility of oil, water, and polar chemicals. But for the development and validation of the model, experimental data are required. This work presents new experimental liquid-liquid equilibrium (LLE) data for 1,2-ethanediol (MEG) + condensate and MEG + water + condensate systems at temperatures from (275 to 323) K at atmospheric pressure. The condensate used in this work is a stabilized natural gas condensate from an offshore field in the North Sea. Compositional analysis of the natural gas condensate was carried out by gas chromatography, and detailed separation of individual condensate's components has been carried out. Approximately 85 peaks eluting before nonane were identified by their retention time. Peak areas were converted to mass fraction using 1-heptene as an internal standard. The components were divided into boiling range groups from hexane to nonane. Paraffinic (P), naphthenic (N), and aromatic (A) distributions were obtained for the boiling point fractions up to nonane. The average molar mass and the overall density of the condensate were measured experimentally. For the mutual solubility of MEG and condensate, approximately 72 component peaks could be detected up to nonane and many components from decane plus carbon fraction. Their solubility was quantified, and the sum was reported as solubility of condensate in MEG. A similar procedure
was adopted for the MEG, condensate, and water system, but because of the presence of water, the solubility of condensate in the polar phase decreases, and some of the components were not detectable. © 2011 American Chemical Society.
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.

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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.

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CO2 Flooding in Chalk Reservoirs

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Publication: Research - peer-review › Conference abstract in proceedings – Annual report year: 2010
The Influence of CO2 Solubility in Brine on Simulation of CO2 Injection Into Water Flooded Reservoir and CO2 WAG

Injection of CO2 into depleted oil reservoirs is not only a traditional way to enhance oil recovery but also a relatively cheaper way to sequester CO2 underground since the increased oil production can offset some sequestration cost. CO2 injection process is often applied to water flooded reservoirs and in many situations alternating injection of water and CO2 is required to stabilize the injection front. Both scenarios involve a large amount of water, making CO2 solubility in brine, which is around ten times higher than methane solubility, a non-negligible factor in the relevant reservoir simulations. In our previous study, a 1-D 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.

General information
State: Published
Organisations: CERE – Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering
Authors: Yan, W. (Intern), Stenby, E. H. (Intern)
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 monooethylene 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.
Coupling Miscible Flow and Geochemistry for Carbon Dioxide Flooding into North Sea Chalk Reservoir

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
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

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

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
Capture and Storage Projects at IVC-SEP

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Center for Energy Resources Engineering, CERE – Center for Energy Resources Engineering, Department of Chemistry
Publication date: 2008
Event: Poster session presented at DTU Energy Conference, Technical University of Denmark, Copenhagen, DK, .
Main Research Area: Technical/natural sciences
Electronic versions:
DTUEnergy_IVCPoster5_2_.pdf
Source: orbit
Source-ID: 232201
Publication: Research - peer-review › Poster – Annual report year: 2008

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
Source: orbit
Source-ID: 236537
Publication: Research - peer-review › Article in proceedings – Annual report year: 2008

Comments on "Measurement and modeling of the solubility of water in supercritical methane and ethane from 310 to 477 K and pressures from 3.4 to 110 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: Kontogeorgis, G. (Intern), Yan, W. (Intern)
Pages: 4347-4348
Publication date: 2007
Main Research Area: Technical/natural sciences

Publication information
Journal: Industrial & Engineering Chemistry Research
Volume: 46
Issue number: 12
ISSN (Print): 0888-5885
Ratings:

BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.1 SJR 0.945 SNIP 1.139
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.949 SNIP 1.146 CiteScore 2.87
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.012 SNIP 1.292 CiteScore 2.85
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 0.982 SNIP 1.243 CiteScore 2.6
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.066 SNIP 1.338 CiteScore 2.56
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.086 SNIP 1.24 CiteScore 2.58
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.047 SNIP 1.165
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.002 SNIP 1.164
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 1.142 SNIP 1.267
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.105 SNIP 1.239
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.035 SNIP 1.204
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 0.993 SNIP 1.241
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 1.046 SNIP 1.452
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 1.101 SNIP 1.266
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 1.191 SNIP 1.183
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 1.256 SNIP 1.346
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 1.372 SNIP 1.41
Web of Science (2000): Indexed yes
Scopus rating (1999): SJR 1.342 SNIP 1.398

Original language: English
DOIs:
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 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)
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 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

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
Interfacial Tension of (Methane + Nitrogen) + Water and (Carbon Dioxide + Nitrogen) + Water Systems

Interfacial tension data of (CH4 + N2) + H2O and (CO2 + N2) + H2O systems were measured using a pendant-drop method. The temperature and pressure ranges were 298-373 K and 1-30 MPa, respectively. The effects of gas composition, temperature, and pressure on the interfacial tension of the systems studied have been investigated. The linear gradient theory (LGT) was used to calculate the interfacial tensions of these two systems. The results show good agreement between the calculated and experimental interfacial tension data for the (CH4 + N2) + H2O system. However, it was found that the LGT model with one adjustable parameter is inadequate to give accurate predictions for the CO2 + H2O system and thus is not suitable for the description of the (CO2 + N2) + H2O system.
Scopus rating (2013): SJR 1.135 SNIP 1.199 CiteScore 2.17
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.141 SNIP 1.103 CiteScore 2.01
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.862 SNIP 0.988 CiteScore 1.8
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.054 SNIP 1.299
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.313 SNIP 1.037
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.505 SNIP 1.186
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.263 SNIP 1.254
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.146 SNIP 1.33
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.155 SNIP 1.342
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 0.897 SNIP 1.205
Scopus rating (2003): SJR 1.054 SNIP 1.157
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 0.661 SNIP 1.062
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 0.978 SNIP 1.234
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 0.735 SNIP 1.16
Scopus rating (1999): SJR 0.891 SNIP 1.249
Original language: English
DOIs:
10.1021/je0101505
Publication: Research - peer-review › Journal article – Annual report year: 2001

Projects:

Characterization of the non-uniform fluid distribution in tight petroleum reservoirs

Department of Chemical and Biochemical Engineering
Period: 01/05/2018 → 30/04/2021
Number of participants: 4
Phd Student:
Baghooee, Hadise (Intern)
Supervisor:
Lassen, Charlotte (Intern)
Yan, Wei (Intern)
Main Supervisor:
Shapiro, Alexander (Intern)
Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)
Project: PhD

Experimental investigation of gas injection processes for enhanced oil recovery
Department of Chemistry
Period: 15/03/2018 → 14/03/2021
Number of participants: 4
PhD Student:
Tagliaferri, Stefano (Intern)
Supervisor:
Shapiro, Alexander (Intern)
Yan, Wei (Intern)
Main Supervisor:
Feilberg, Karen Louise (Intern)

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

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

Analysis of reservoir water samples and injected sea water for enhanced oil recovery
Department of Chemistry
Period: 01/11/2016 → 31/10/2019
Number of participants: 3
PhD Student:
Nitsche Gottfredsen, Sofie (Intern)
Supervisor:
Yan, Wei (Intern)
Main Supervisor:
Feilberg, Karen Louise (Intern)

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

Estimation of Matrix Flow contribution in naturally fractured reservoirs
Department of Chemical and Biochemical Engineering
Application of an association equation of state to enhanced oil recovery processes

Department of Chemical and Biochemical Engineering
Period: 01/05/2015 → 30/06/2018
Number of participants: 3
Phd Student:
Pinto Coelho Muniz Vinhal, Andre (Intern)
Supervisor:
Yan, Wei (Intern)
Main Supervisor:
Kontogeorgis, Georgios (Intern)
Examiner:
Jessen, Kristian (Intern)
Solbraa, Even (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Science Without Borders, Brasi
Project: PhD

Computation of Simultaneous Phase and Chemical Equilibrium

Department of Chemistry
Period: 15/12/2014 → 15/01/2018
Number of participants: 6
Phd Student:
Tsanas, Christos (Intern)
Supervisor:
Stenby, Erling Halfdan (Intern)
Main Supervisor:
Yan, Wei (Intern)
Examiner:
Kontogeorgis, Georgios (Intern)
Jessen, Kristian (Intern)
Solbraa, Even (Ekstern)

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

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:
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

Modeling of Asphaltene systems with Association Models

Department of Chemical and Biochemical Engineering
Period: 01/01/2014 → 26/04/2017
Number of participants: 6
Phd Student:
Arya, Alay (Intern)
Supervisor:
von Solms, Nicolas (Intern)
Main Supervisor:
Kontogeorgis, Georgios (Intern)
Examiner:
Yan, Wei (Intern)
Serensen, Henrik (Ekstern)
Vargas, Francisco M. (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: 1/3 FUU, 1/3 inst 1/3 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

Enhanced Oil Recovery with Application of Microorganisms

Department of Chemical and Biochemical Engineering
Period: 01/02/2012 → 01/07/2015
Number of participants: 7
Phd Student:
Halim, Amalia Yunita (Intern)
Supervisor:
Eliasson Lantz, Anna (Intern)
Nielsen, Sidsel Marie (Intern)
Main Supervisor:
Shapiro, Alexander (Intern)
Examiner:
Yan, Wei (Intern)
Alkan, Hakan (Ekstern)
Zahid, Adeel (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: 1/3 FUU, 1/3 inst 1/3 Andet
Project: PhD

Enhanced Oil Recovery with Application of Enzymes

Department of Chemical and Biochemical Engineering
Period: 01/12/2011 → 26/05/2016
Number of participants: 6
Phd Student:
Khusainova, Alsu (Intern)
Supervisor:
Woodley, John (Intern)
Main Supervisor:
Shapiro, Alexander (Intern)
Examiner:
Yan, Wei (Intern)
Ivar Andersen, Simon (Intern)
Skauge, Arne (Ekstern)

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

Relations
Publications:
Enhanced Oil Recovery with Application of Enzymes
Project: PhD

Thermodynamic modelling in oil-sea water mixtures
Department of Chemical and Biochemical Engineering
Period: 15/08/2011 → 26/11/2014
Number of participants: 7
Phd Student:
Liang, Xiaodong (Intern)
Supervisor:
Thomsen, Kaj (Intern)
Yan, Wei (Intern)
Main Supervisor:
Kontogeorgis, Georgios (Intern)
Examiner:
von Solms, Nicolas (Intern)
Lindeloff, Niels (Intern)
Sadowski, Gabriele (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: 1/3 FUU, 1/3 inst 1/3 Andet
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

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

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**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

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**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
Project: PhD

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