Modeling the influence of potassium content and heating rate on biomass pyrolysis

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

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Comparative analysis of experimental methods for quantification of small amounts of oil in water
During core flooding experiments where water is injected into oil bearing core plugs, the produced fluids can be sampled in a fraction collector. When the core approaches residual oil saturation, the produced amount of oil is typically small (can be less than a few microliters) and the quantification of oil is then difficult. In this study, we compare four approaches to determine the volume of the collected oil fraction in core flooding effluents. The four methods are: Image analysis, UV/visible spectroscopy, liquid scintillation counting, and low-field nuclear magnetic resonance (NMR) spectrometry. The procedure followed to determine the oil fraction and a summary of advantages and disadvantages of each method are given. Our results show that all four methods are reproducible with high accuracy. The NMR method was capable of direct quantification of both oil and water fractions, without comparison to a pre-made standard curve. Image analysis, UV/visible spectroscopy, and liquid scintillation counting quantify only the oil fraction by comparing with a pre-made standard curve. The image analysis technique is reliable when more than 0.1 ml oil is present, whereas liquid scintillation counting performs well when less than 0.6 ml oil is present. Both UV/visible spectroscopy and NMR spectrometry produced high accuracy results in the entire studied range (0.006-1.1 ml). In terms of laboratory time, the liquid scintillation counting is the fastest and least user dependent, whereas the NMR spectrometry is the most time consuming. (C) 2016 Elsevier B.V. All rights reserved.

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Enhanced Oil Recovery with Application of Enzymes

Enzymes have recently been reported as effective enhanced oil recovery (EOR) agents. Both laboratory and field tests demonstrated significant increase in the ultimate oil production. Up to 16% of additional oil was produced in the laboratory conditions and up to 269 barrels of additional oil per day were recovered in the field applications. The following mechanisms were claimed to be responsible for the enhancement of the oil production due to enzymes: wettability improvement of the rock surface; formation of the emulsions; reduction of oil viscosity; and removal of high molecular weight paraffins. However, the positive effect of enzymes on oil recovery is not that obvious. In most of the studies commercial enzyme products composed of enzymes, surfactants and stabilisers were used. Application of such samples makes it difficult to assign a positive EOR effect to a certain compound, as several components of commercial mixture might possess surface-active properties. Hence, the main goals of the present study were to establish whether enzymes alone can improve oil production and to identify mechanisms that might underlie enzymatic EOR (EEOR), especially,
under conditions of the North Sea petroleum reservoirs. At the first stage of the work enzyme samples that might have potential for EOR applications were selected. Wettability tests such as measurements of contact angles and determination of adhesion behaviour were applied as screening tools. The group of lipases/esterases demonstrated strong ability to detach oil from the calcite surface and was identified as the most promising group for further investigations. Wettability improvement due to protein adsorption on to the mineral was proposed as the main mechanism for EEOR. It was also proved that the enzyme molecules themselves caused change of the wetting state of calcite, while presence of stabilising ingredients did not interfere the results. Implementation of such a mechanism of enzymatic action under reservoir conditions might be limited by retention of the protein molecules in the porous medium. In order to verify this hypothesis, adsorption behaviour of enzymes/proteins on the reservoir rocks was studied by application of the static adhesion tests and adsorption experiments on powders, as well as dynamic flow-through experiments. It was established that enzymes are indeed significantly lost during the transport in the porous media due to the irreversible adsorption. The adsorption capacity of carbonate material was found to be much higher compared to sandstone. Various methods (forexample, change of ionic strength and pH of the enzyme solution and displacing fluid) were applied in order to desorb attached protein molecules, but no desorption was observed. Another possible mechanism that might underlie EEOR is formation of enzyme-stabilised emulsions. Similar to the wettability screening, lipases/esterases demonstrated the best surface active properties: they formed the most stable emulsions with rather small drops. Light fractions of the crude oil participated mostly in formation of the protein-stabilised emulsions. Incubation of the oil-[enzyme + sea water] systems was found to be important in order to obtain high stability of emulsions. Combined application of enzymes and solid particles was an alternative way to increase emulsion stability. Other crude oil-brine interaction tests revealed additional problems that can rise during the application of enzymatic EOR. Interaction of the enzyme solution with the crude oil can induce gelation/emulsification of the propylene glycol (the main component of the enzyme productstabilisers). Moreover, when purified enzyme containing almost no stabilisers was used, a highly viscous oil-in-water emulsion was formed. Finally, assessment of enzymes as EOR agents under conditions similar to the conditions of the petroleum reservoirs was carried out in core flooding experiments. Two types of enzymes(lipase and amylase) were selected based on the results from the wettability and emulsion studies. They were only tested in tertiary mode, employing various injection schemes. Application of enzymes in sandstone core samples resulted in increase of the ultimate oil production by 0.23-1.69% relative to original oil in place, while no additional oil due to enzymes was produced from chalk. Wettability change was confirmed to be the main EOR mechanism, while emulsification plays less significant role. Overall, enzymes have possessed low potential for EOR applications at least in sandstone and chalk reservoirs containing light crude oils. An alternative technique that will shift adsorption balance towards reversible adsorption should be established in order to make enzymatic EOR an effective and economically feasible oil recovery method.

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**Fast pyrolysis of biomass at high temperatures**

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

The differences in the char yield for particle size fractions in the range of 0.05 mm were negligible, leading to the conclusion that the biomass particle can be assumed isothermal, when its size did not exceed 0.425 mm. Compared to smaller particles, the larger pinewood particles (d > 0.85 mm) required more than 1 s holding time for the complete conversion at intermediate and fast heating rates. The influence of heating rate on the char yield was less pronounced for larger particles (from 0.85 to 4 mm) obtained at temperatures > 1250°C in the wire mesh reactor, single particle burner and drop tube reactor, due to the predominance of internal heat transfer control within the large particles.

Potassium compared to all other ash elements in the fuels had the highest influence on the char yield. The effect of potassium on the char yield was stronger at low and intermediate heating rates where potassium catalyzed the repolymerization and cross-linking reactions, leading to higher char yields. Silicon compounds abundant in herbaceous biomass had a negligible influence on the char yield and reactivity. However, a very high content of silicon oxides in biomass (> 50% of the overall biomass inorganic matter) significantly affected the char morphology, as observed for rice husk. For this fuel, the high content of low-temperature melting amorphous silicon oxides led to the formation of a glassy shell on rice husk chars at 1000-1500°C. The ability of char to melt in fast pyrolysis followed the order pinewood > beechwood, straw > rice husk, and was related to the formation of metaplast. Different particle shapes of beechwood and leached wheat straw chars produced in the drop tube reactor which have similar potassium content suggested a stronger influence of the major biomass cell wall compounds (cellulose, hemicellulose, lignin and extractives) and silicates on the char morphology than alkali metals. In this study, potassium lean pinewood (0.06 wt. %) produced the highest soot yield (9 and 7 wt. %) at 1250 and 1400°C, whereas leached wheat straw with the higher potassium content (0.3 wt. %) generated the lowest soot yield (2 and 1 wt. %). Soot yields of wheat and alfalfa straw at both temperatures were 5% points lower than wood soot yields and 3% points higher than leached wheat straw soot yield, indicating that potassium plays a minor role on the soot formation. The leaching of alkali from wheat straw additionally resulted in a removal of lignin, leading to the decreased formation of polycyclic aromatic hydrocarbon precursors, and thereby to lower soot yields. Pinewood soot particles produced at 1250°C were significantly larger (77.7 nm) than soot particles produced in pinewood (47.8 nm) pyrolysis at 1400°C, beechwood (43 nm) and wheat straw (30.8 nm) devolatilization at both temperatures. The larger pinewood soot particles were related to the formation of tar balls known from smoldering combustion. The major difference in nanostructure of pinewood, beechwood and wheat straw soot was in the formation of multi and single core particles. Pinewood soot particles generated at 1250°C were mainly multi core structures compared to pinewood soot generated at 1400°C, combining both single and multi core particles. Beechwood and wheat straw soot samples had multi and single core particles at both temperatures. In thermogravimetric analysis, the maximal reaction rate of pinewood soot was shifted to temperatures about 100°C higher than for the other samples in both oxidation and CO₂ gasification, indicating a significantly lower reactivity. Soot samples produced at 1400°C were more reactive than soot generated at 1250°C. The beechwood and wheat straw soot samples were more graphitic than pinewood soot based on the electron energy loss spectroscopy (EELS) analysis. In contrast to expectations of graphitic structures to react slower than amorphous samples, beechwood and wheat straw soot were 35 and 571 times more reactive than pinewood soot prepared at 1400°C.

The presence of potassium in wheat straw soot mainly as water-soluble KCl, KOH, KHCO₃ and K₂CO₃ and to a minor extent bonded to the soot matrix in oxygen-containing surface groups (e.g. carboxyl, phenolate) or intercalated in soot graphene layers led to a higher reactivity in CO₂ gasification compared to low-alkali containing pinewood soot. The results showed that potassium has a dominating effect on the soot reactivity compared to nanostructure and particle size. A mathematical model of biomass fast pyrolysis was developed to predict the gas and char yield of wood and herbaceous biomass at heating rates > 600 K s⁻¹. The model includes both kinetics and external and internal heat transfer assuming that mass transfer is fast. The model relies on the concept applied in fast pyrolysis of cellulose through the formation of an intermediate liquid (so-called metaplast) which reacts further to form char and gas. The kinetics of the fast pyrolysis was described through the Broido-Shafizadeh scheme for biomass. The catalytic effect of potassium which is a major ash element influencing the char yield was included in the model.
Mechanics of the Separating Surface for a Two-Phase Co-current Flow in a Porous Medium

A mechanical description of an unsteady two-phase co-current flow in a porous medium is developed based on the analysis of the geometry and motion of the surface separating the two phases. It is demonstrated that the flow should be considered as essentially three-dimensional, even if the phase velocities are co-directed, since the phase interface is on average inclined to the direction of the flow. Kinematics of the flow is described, distinguishing between the average velocities of the bulk phases and their velocity near the interface between them. Dynamics of the flow is analyzed by means of the extended Maxwell-Stefan formalism, as in our previous paper (Shapiro 2015). Force balances are formulated in the directions parallel and orthogonal to the flow. A complete system of the flow equations, generalizing the traditional Buckley–Leverett and Rappoport–Leas system, is derived. Sample computations show that one of the main effects produced by the new system is sharpening of the displacement front, which otherwise would be washed out by the capillary forces, as in the solution of the Rappoport–Leas equation.
Microbial enhanced oil recovery—a modeling study of the potential of spore-forming bacteria

Microbial enhanced oil recovery (MEOR) utilizes microbes for enhancing the recovery by several mechanisms, among which the most studied are the following: (1) reduction of oil-water interfacial tension (IFT) by the produced biosurfactant and (2) selective plugging by microbes and metabolic products. One of the ways of bacterial survival and propagation under harsh reservoir conditions is formation of spores. A model has been developed that accounts for bacterial growth, substrate consumption, surfactant production, attachment/filtering out, sporulation, and reactivation. Application of spore-forming bacteria is an advantageous novelty of the present approach. The mathematical setup is a set of 1D transport equations involving reactions and attachment. Characteristic sigmoidal curves are used to describe sporulation and reactivation in response to substrate concentrations. The role of surfactant is modification of the relative permeabilities by decreasing the interfacial tension. Attachment of bacteria reduces the pore space available for flow, i.e., the effective porosity and permeability. Clogging of specific areas may occur. An extensive study of the MEOR on the basis of the developed model has resulted in the following conclusions. In order to obtain sufficient local concentrations of surfactant, substantial amounts of substrate should be supplied; however, massive growth of bacteria increases the risk for clogging at the well inlet areas, causing injectivity loss. In such areas, starvation may cause sporulation, reducing the risk of clogging. Substrate released during sporulation can be utilized by attached vegetative bacteria and they will continue growing and producing surfactant, which prolongs the effect of the injected substrate. The simulation scenarios show that application of the spore-forming bacteria gives a higher total production of surfactant and the reduced risk of clogging, leading to an increased period of production and a higher oil recovery.
Investigation of spore forming bacterial flooding for enhanced oil recovery in a North Sea chalk Reservoir

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

**General information**

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Organisations: Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering, Maersk Oil and Gas A/S

Authors: Halim, A. Y. (Intern), Nielsen, S. M. (Intern), Eliasson Lantz, A. (Intern), Sander Suicmez, V. (Ekstern), Lindeloff, N. (Ekstern), Shapiro, A. (Intern)

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Web of Science (2006): Indexed yes

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Scopus rating (2004): SJR 0.823 SNIP 1.302

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Modeling of Dissolution Effects on Waterflooding

Physico-chemical interactions between the fluid and reservoir rock due to the presence of active components in the injected brine produce changes within the reservoir and can significantly impact the fluid flow. We have developed a 1D numerical model for waterflooding accounting for dissolution and precipitation of the components. Extending previous studies, we consider an arbitrary chemical non-equilibrium reaction-induced dissolution. We account for different individual volumes that a component has when precipitated or dissolved. This volume non-additivity also affects the pressure and the flow rate. An equation of state is used to account for brine density variation with regard to pressure and composition.

We present a numerical study of the evolution of the reservoir parameters in the framework of the developed model. It is demonstrated that the systems characterized by large Damkohler numbers (fast reaction rates) may exhibit rapid increase of porosity and permeability near the inlet probably indicating a formation of high permeable channels (wormholes). Water saturation in the zone of dissolution increases due to an increase in the bulk volume accessible for the injected fluid. Volumetric non-additivity is found to be responsible for insignificant change in the velocity of the displacement front.

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Modeling of Salinity Effects on Waterflooding of Petroleum Reservoirs

Smart water flooding is an enhanced oil recovery (EOR) technique that is based on the injection of chemistry-optimized water with changed ionic composition and salinity into petroleum reservoirs. Extensive research that has been carried out over the past two decades has clearly demonstrated that smart water flooding can improve the ultimate oil recovery both in carbonate and sandstone reservoirs. A number of different physicochemical mechanisms of action were proposed to explain the smart water effects, but none of them has commonly been accepted as a determining mechanism. Most of the experimental studies concerning the smart water effects recognize importance of the chemistry of reservoir rocks that manifests itself in dissolution and precipitation of rock minerals and adsorption of specific ions on the rock surface. The brine-rock interactions may affect the wetting state of the rock and in some cases result in mobilization of the trapped oil.

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

Further, we study the mechanisms that can govern the mobilization of residual oil and its flow in porous media. The oil trapped in the swept zones after conventional flooding is present in a form of disconnected oil drops, or oil ganglia. While the macroscopic theory of multiphase flow assumes that fluid phases flow in their own pore networks and do not influence each other, the flow of disconnected oil ganglia requires an alternative description. We address this problem by
considering a micromodel for the two-phase flow in a single angular pore-body. On the micro-level, both fluids can be present in a single pore body and interact during the flow. Considering water-wet systems, we find that presence of the water on the surface of the rock and in the corner filaments of pore bodies results in a larger velocity of the viscous flow of the oil phase due to the increased area of the moving oil-water interface. Moreover, the flow of oil may be induced solely by the action of viscous forces at the oil-water interface, which appears to be a new mechanism for the transport of disconnected oil ganglia in porous media. We derive correlations that allow calculating the flow velocities of fluid phases in single pore bodies based on the pore fluid saturations. Based on the microscale considerations, we develop a macroscopic model of displacement accounting for the effects associated with oil ganglia. The model is based on the assumption that wettability alteration toward increased water-wetness caused by the presence of active species in the injected brine results in formation of the wetting films on the surface of the rock. Oil ganglia are mobilized and carried by the slow flow of wetting films. Considering simplistc pore-network model, we derive the macroscopic system of equations involving description of the transport of oil ganglia. As a result of numerical modeling of the tertiary recovery process, it is found that production of oil ganglia may continue for a long time of injection of around 10 to 20 PVI.

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

One of the possible chemical mechanisms through which the mobilization of the residual oil may occur in carbonates is alteration of the electrostatic potential of the surface. Reduction of the surface charge due to adsorption of the potential determining ions results in the decrease in oil affinity towards the surface of the rock. We establish a mathematical model that takes into account adsorption of the potential determining ions: calcium, magnesium, and sulfate, on the chalk surface, to investigate how the composition of the injected brine affects the equilibrium surface composition and how adsorption process affects the composition of the produced brine. We use experimental data on the produced brine composition from the flow-through experiments to estimate the parameters of the adsorption model. The computations suggest that there is no evidence of usually assumed stronger adsorption of magnesium ion compared to calcium at high temperatures. In order to investigate the effect of surface composition on the flooding efficiency, we combine the adsorption model with the Buckley-Leverett model and perform simulations of the experiments concerning flooding in the water-wet outcrop chalk. Computations of the equilibrium surface composition demonstrate a correlation between the concentration of the adsorbed sulfate and the ultimate recovery observed in the experiments indicating that a more negatively charged surface of chalk could be a factor that affects the recovery efficiency without wettability modification.

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Multicomponent Adsorption Model for Polar and Associating Mixtures
The multicomponent potential adsorption theory (MPTA) is revisited in this work for polar and associating systems. MPTA is used in combination with the CPA equation of state. Previous Studies have shown that both MPTA and other theories present difficulties for complex systems. Some of these problems could be due to the fact that the original MPTA assumes that a given adsorbent has the same adsorption capacity (for example, porous volume) for all the adsorbed substances and is adjusted simultaneously to many data. This is a simplified picture, as experimental data indicate that the adsorption capacities of the various components may also differ. In this paper we develop a scheme for the distribution of the potential, which accounts for the presence of the porous space occupied either by just one component or by both components. These capacities are determined by adjustment of the potentials to experimental data on single-component adsorption. We show that MPTA involving the different adsorption capacities for the different components is capable of
predicting binary adsorption data for most of the mixtures considered. In our application of MPTA, we used both the well-known Dubinin-Radushkevich-Astakhov potentials and the potentials directly restored from experimental data by solving the inverse problem. Application of the latter potentials clearly demonstrates the importance of the difference in adsorption capacities. However, the quality of prediction of binary adsorption is similar for both potentials. Thus, we feel that there is no need to use more complex potentials provided that the difference in the individual adsorption capacities is accounted for.

**General information**
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Organisations: Center for Energy Resources Engineering, Department of Chemistry, Physical and Biophysical Chemistry, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering
Authors: Nesterov, I. (Intern), Shapiro, A. (Intern), Kontogeorgis, G. M. (Intern)
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Scopus rating (2014): SJR 1.012 SNIP 1.292 CiteScore 2.85
Web of Science (2014): Indexed yes
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Scopus rating (2012): SJR 1.066 SNIP 1.338 CiteScore 2.56
Web of Science (2012): Indexed yes
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Scopus rating (2010): SJR 1.047 SNIP 1.165
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BFI (2008): BFI-level 2
Scopus rating (2008): SJR 1.142 SNIP 1.267
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Scopus rating (2007): SJR 1.105 SNIP 1.239
Optimization of Spore Forming Bacteria Flooding for Enhanced Oil Recovery in North Sea Chalk Reservoir

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

Quantification of the recovered oil and water fractions during water flooding laboratory experiments

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

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Organisations: Department of Civil Engineering, Section for Geotechnics and Geology, Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering
Authors: Katika, K. (Intern), Halim, A. Y. (Intern), Shapiro, A. (Intern), Fabricius, I. L. (Intern)
Number of pages: 5
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Study of wettability of calcite surfaces using oil-brine-enzyme systems for enhanced oil recovery applications
Enzymes have recently been considered as possible agents for enhanced oil recovery (EOR) acting at the liquid-solid interface. One way to assess this is via measuring the wettability of calcite surfaces, important for EOR methods in carbonaceous reservoirs. In the present work, we have experimentally investigated the effect of enzymes on the wettability of calcite mineral surfaces with oil-brine systems. The action of various enzymes, including esterases/lipases, carbohydrates, proteases and oxidoreductases (along with two commercial mixtures) was studied by contact angle measurements and adhesion behaviour tests. Comparative studies with a surfactant, protein, purified enzyme, enzyme stabiliser using n-decane (as a model for the oil) have also been carried out in order to verify experimental results. The enzymes that have the highest effect on the wettability have been identified. Those enzymes, which were found the most promising from a practical perspective, have shown the ability to fully detach oil from the surface, even at very low enzyme concentrations. For example, esterases/lipases were found to strongly affect the wettability and to remove adhesion at concentrations as low as 0.1% of the enzyme product (corresponding to 0.002-0.005% protein). Likewise, proteases could also improve wettability, although the effect was not consistent and was dependent on impurities. Other enzymes had no effect on the wettability of calcite at the concentration studied. The main mechanism of enzymatic action has been found to be replacement of oil at the solid surface by the enzyme. Other mechanisms (modification of the surface tension or catalytic modification of hydrocarbons resulting in reducing the oil viscosity) have shown to be much less pronounced from the measurements reported here.

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Organisations: Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering, CAPEC-PROCESS, Technical University of Denmark, Novozymes A/S
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Scopus rating (2016): CiteScore 2.56 SJR 0.764 SNIP 1.631
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.801 SNIP 1.652 CiteScore 2.38
Web of Science (2015): Indexed yes

We develop an approach to coupling between viscous flows of the two phases in porous media, based on the Maxwell–Stefan formalism. Two versions of the formalism are presented: the general form, and the form based on the interaction of the flowing phases with the interface between them. The last approach is supported by the description of the flow on the mesoscopic level, as coupled boundary problems for the Brinkmann or Stokes equations. It becomes possible, in some simplifying geometric assumptions, to derive exact expressions for the phenomenological coefficients in the Maxwell–Stefan transport equations. Sample computations show, among other, that apparent relative permeabilities are dependent on the viscosity ratio; that the overall mobility of the phases decreases compared to the standard Buckley–Leverett formalism; and that the effect is determined by the parameter determining the “degree of mixing” between the flowing phases. Comparison to the available experimental data on the steady-state two-phase relative permeabilities is presented.
Crossflow and water banks in viscous dominant regimes of waterflooding

Understanding the crossflow in multilayered reservoirs is of great importance for designing mobility control methods for enhanced oil recovery. The authors reveal saturation profiles in stratified reservoirs to study the interlayer communication in the viscous dominant regime. The displacement profiles are more even and smoother in a communicating layer-cake reservoir than in a noncommunicating one. Water banks and transition zones may be observed. Analysis indicates that the phenomena are attributed to the enhanced crossflow due to large mobility ratios (water-oil). The mobility control techniques that take advantage of crossflow between layers may be more efficient with large mobility ratios. © 2014 Copyright Taylor & Francis Group, LLC.
Experimental Study of Bacterial Penetration into Chalk Rock: Mechanisms and Effect on Permeability

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

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Organisations: Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering, Department of Systems Biology, Metabolic Signaling and Regulation
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Simulations of Microbial-Enhanced Oil Recovery: Adsorption and Filtration

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

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Organisations: Center for Energy Resources Engineering, Department of Chemistry, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering
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Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.728 SNIP 1.317 CiteScore 1.94
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.932 SNIP 1.433 CiteScore 1.91
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.04 SNIP 1.433 CiteScore 2.03
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.942 SNIP 1.522 CiteScore 1.88
ISI indexed (2012): ISI indexed yes
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BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.921 SNIP 1.337 CiteScore 1.81
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.615 SNIP 1.203
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.612 SNIP 1.088
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.7 SNIP 0.924
Scopus rating (2007): SJR 0.717 SNIP 1.215
A Theoretical Analysis of Colloid Attachment and Straining in Chemically Heterogeneous Porous Media

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

General information

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Organisations: Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering, US Salinity Laboratory, Commonwealth Scientific and Industrial Research Organisation
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Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.99 SJR 1.55 SNIP 1.188
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.686 SNIP 1.308 CiteScore 4.33
Multicomponent adsorption of gas mixtures on diverse solid surfaces is important in many applications. However, there are still many questions on the practical applicability of the available theories, especially for polar systems. In this work, we consider three well-known theories suitable for the prediction of multicomponent adsorption with parameters obtained solely from correlating single gas/solid data. We have tested them over an extensive database with emphasis on polar systems (both gases and solids). The three theories are the multicomponent Langmuir, the ideal adsorbed solution theory (IAST), and the multicomponent potential adsorption theory (MPTA). We have not attempted to improve/modify the...
methods in any way but have used them in their original form, as the purpose of our work is to illustrate the capabilities and inherent limitations of the models for predicting multicomponent adsorption. We have ensured that the description of single gas/solid systems is as accurate as possible, but besides this, the calculations for multicomponent systems are straight predictions. The work revealed on one side that all three theories yield for some systems similar predictions, with IAST and MPTA performing overall better than the multicomponent Langmuir. On the other hand, it is also shown that all the three theories, despite the good results in some cases, have serious limitations particularly for water and to some extent also for certain polar solids. Both strengths and weaknesses of the three models are discussed. © 2013 American Chemical Society.

General information
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Organisations: Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering, Haldor Topsoe AS, Statoil ASA
Authors: Bartholdy, S. (Ekstern), Bjørner, M. G. (Intern), Solbraa, E. (Ekstern), Shapiro, A. (Intern), Kontogeorgis, G. (Intern)
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Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.012 SNIP 1.292 CiteScore 2.85
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 0.982 SNIP 1.243 CiteScore 2.6
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
Improved population balance model for straining-dominant deep bed filtration using network calculations

Colloidal-suspension flow in porous media is modelled simultaneously by the large scale population balance equations and by the microscale network model. The phenomenological parameter of the correlation length in the population balance model is determined from the network modelling. It is found out that the correlation length in the population balance model depends on the particle size. This dependency calculated by two-dimensional network has the same tendency as that obtained from the laboratory tests in engineered porous media.

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Organisations: Center for Energy Resources Engineering, CERE – Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, University of Adelaide
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Web of Science (2017): Indexed yes
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Scopus rating (2016): CiteScore 6.34
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 5.68
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Molasses injection as a MEOR strategy: Enrichment incubations of brine/oil from North Sea Oil Field

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Organisations: Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering, Department of Systems Biology, Metabolic Signaling and Regulation, Danish Technological Institute
Authors: Halim, A. Y. (Intern), Pedersen, D. S. (Ekstern), Eliasson Lantz, A. (Intern), Nielsen, S. M. (Intern), Shapiro, A. (Intern)
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Numerical analysis of a one-dimensional multicomponent model of the in-situ combustion process

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

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Organisations: Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering, Department of Chemistry
Authors: Nesterov, I. (Intern), Shapiro, A. (Intern), Stenby, E. H. (Intern)
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Scopus rating (2016): CiteScore 2.56 SJR 0.764 SNIP 1.631
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BFI (2015): BFI-level 1
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Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.692 SNIP 1.751 CiteScore 1.95
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.822 SNIP 1.901 CiteScore 1.73
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.774 SNIP 1.666 CiteScore 1.42
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.648 SNIP 1.41 CiteScore 1.29
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.746 SNIP 1.724
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.072 SNIP 1.852
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.841 SNIP 1.435
Scopus rating (2007): SJR 0.732 SNIP 1.386
Scopus rating (2006): SJR 0.92 SNIP 1.387
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 0.784 SNIP 1.052
Potential theory of adsorption for associating mixtures: possibilities and limitations

The applicability of the Multicomponent Potential Theory of Adsorption (MPTA) for prediction of the adsorption equilibrium of several associating binary mixtures on different industrial adsorbents is investigated. In the MPTA the adsorbates are considered to be distributed fluids subject to an external potential field emitted by the adsorbent. In this work, the theory is extended to include the Cubic-Plus-Association (CPA) equation of state (EoS), for the description of the fluid-fluid interactions of associating mixtures. The Dubinin-Radushkevich-Astakhov (DRA) potential function is utilized to describe the solid-fluid interactions. The potential is extended to include adsorbate-absorbent specific capacities rather than an adsorbent specific capacity. Correlations of pure component isotherms are generally excellent with individual capacities, although adsorption on silicas at different temperatures still poses a challenge. The quality of the correlations is usually independent on the applied EoS. Predictions for binary mixtures indicate that the MPTA+SRK is superior when adsorption occurs on non-polar or slightly polar adsorbents, while MPTA+CPA performs better for polar adsorbents, or when the binary mixtures only contain associating compounds. Predictions are typically improved by about 3% when individual capacities are employed, but improvements can in some cases be as large as 45%. When individual capacities and the best performing EoS are used, average absolute deviations of the selectivity are as low as 7-12%. Predictions of the selectivity are generally superior to predictions of the adsorbed amounts. The sensitivity of the model has also been tested, and it is concluded, that predictions are very sensitive to the adsorption energies.

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Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.012 SNIP 1.292 CiteScore 2.85
Solving inverse problems through a smooth formulation of multiple-point geostatistics

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

The Effect of Bacteria Penetration on Chalk Permeability

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

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General information
State: Published
Organisations: National Space Institute, Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering, Department of Chemistry
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The Effect of Bacteria Penetration on Chalk Permeability
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General information
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A New Comprehensive Approach for Predicting Injectivity Decline during Waterflooding

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

General information
State: Published
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Application of Stochastic Approaches to Modelling Suspension Flow in Porous Media

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

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Colloid Transport and Retention: Recent Advances in Colloids Filtration Theory

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

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Estimating filtration coefficients for straining from percolation and random walk theories

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

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Pages: 63-73
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Experimental studies of low salinity water flooding in carbonate reservoirs: A new promising approach

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

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

General information
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Managing Injected Water Composition To Improve Oil Recovery: A Case Study of North Sea Chalk Reservoirs

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

Colloid flow, filtration, and migration in porous media are widely observed in important natural and industrial processes, such as pathogen (bacteria) spreading in aquifers, colloid-facilitated migration of heavy metal in soils, mud filtration during drilling wells, injectivity decline during water injection, and deep bed filtration during waste water treatment. The current thesis aims at better understanding the transport and fate of colloids in porous media. A number of methodologies have been applied in this study, such as developing new mathematical models for colloid filtration, comparing the modeling results to experimental observations, uncertainty and sensitivity analysis of the new models, and realizing the pore-scale physics in network models.

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

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

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

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

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

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

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

General information
State: Published
Organisations: Center for Energy Resources Engineering, CERE – Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, Department of Chemistry
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 ion 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 crude oil at high temperature and pressure. Experimental results indicate that crude oils interact differently with the same brine solutions regarding phase behavior and viscosity measurements. This difference is attributed to the difference in composition of the different crude oils. More experiments are carried out in order to understand mechanisms of the crude oil viscosity reduction and emulsion formation. We observed that a heavy oil (that with a large fraction of heavy components) exhibited viscosity reduction in contact with brine, while a light crude oil exhibited emulsion formation.

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

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

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

Enzymes are well-known biological agents and have been applied previously in petroleum industry. However, only recently they have been introduced into the field of enhanced oil recovery (EOR). Although initially reported results of the application of enzymes for EOR are quite positive and promising (Nasiri et al., 2009), working mechanisms are poorly known and understood. The main goal of the present work is to establish possible mechanisms in which enzymes may enhance oil recovery.

Improvement of the brine wettability of the rock and decrease of oil adhesion to it by addition of an enzyme is one of the possible mechanisms of enzymatic action. This mechanism has been investigated experimentally, by measurements of the contact angles between oil drops and enzyme solutions in brine on the mineral surfaces.

Fifteen enzyme samples belonging to different enzyme classes, such as esterases/lipases, carbohydrases, proteases and oxidoreductases, provided by Novozymes, have been investigated. Two commercial mixtures containing enzymes: Apollo-GreenZyme™ and EOR-ZYMAX™ have also been applied. The North Sea dead oil and the synthetic sea water were used as test fluids. Internal surface of a carbonate rock has been mimicked using calcite crystals.

Overall, the group of esterases/lipases has demonstrated the best performance in terms of wettability alteration. Particularly, a non-specific esterase product has been found to turn the mineral surfaces into non-adhesive state at concentrations of 0.1-0.5% wt. Proteases appear to be relatively ambiguous, while carbohydrases and oxidoreductases have the lowest potential for EOR in the light of the present experiments. Suggested mechanisms for wettability improvement for esterases/lipases are adsorption of enzymes onto the mineral and/or formation of additional interfacially active oil compounds. Application of the commercial product Apollo-GreenZyme™ has also resulted in positive wettability changes, but according to the observations the working mechanisms are different. In an attempt to assess validity of the proposed mechanisms, the reference experiments have been conducted with concentrated enzymes, enzyme product stabilizers, surfactant and protein.
Advanced waterflooding in chalk reservoirs: Understanding of underlying mechanisms

Over the last decade, a number of studies have shown SO42−, Ca2+ and Mg2+ to be potential determining ions, which may be added to the injected brine for improving oil recovery during waterflooding in chalk reservoirs. However, the understanding of the mechanism leading to an increase in oil recovery is still not clear. In this work the crude oil/seawater ions interaction at different temperatures, pressures and sulfate ion concentrations is investigated. Our results show that sulfate ions may help decrease the crude oil viscosity when brine is contacted with oil under high temperature and pressure. We have also observed formation of a microemulsion phase between brine and oil with the increase in sulfate ion concentration at high temperature and pressure. In addition, sulfate ions can reduce interfacial tension (IFT) between oil and water. We propose that the decrease in viscosity and formation of a microemulsion phase could be the possible reasons for the observed increase in oil recovery with sulfate ions at high temperature in chalk reservoirs besides the mechanism of the rock wettability alteration, which has been reported in most previous studies.
A Mathematical Model for Non-monotonic Deposition Profiles in Deep Bed Filtration Systems

A mathematical model for suspension/colloid flow in porous media and non-monotonic deposition is proposed. It accounts for the migration of particles associated with the pore walls via the second energy minimum (surface associated phase). The surface associated phase migration is characterized by advection and diffusion/dispersion. The proposed model is able to produce a nonmonotonic deposition profile. A set of methods for estimating the modeling parameters is provided in the case of minimal particle release. The estimation can be easily performed with available experimental information. The numerical modeling results highly agree with the experimental observations, which proves the ability of the model to catch a non-monotonic deposition profile in practice. An additional equation describing a mobile population behaving differently from the injected population seems to be a sufficient condition for producing non-monotonic deposition profiles. The described physics by the additional equation may be different in different experimental settings.

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BFI (2015): BFI-level 2
There is a considerable and ongoing effort aimed at understanding the transport and the deposition of suspended particles in porous media, especially non-Fickian transport and non-exponential deposition of particles. In this work, the influential parameters in filtration models are studied to understand their effects on the non-Fickian transport and the non-exponential deposition. The filtration models are validated by the comparisons between the modelling results and the experimental data. The elliptic equation with distributed filtration coefficients may be applied to model non-Fickian transport and hyperexponential deposition. The filtration model accounting for the migration of surface associated particles may be applied for non-monotonic deposition.
Induced migration of fines during waterflooding in communicating layer-cake reservoirs
The effects of fines migration induced by injection of water with a different salinity than the reservoir brine are incorporated into the upscaling model for waterflooding in a layer cake reservoir with good communication between the layers. Mobilization and re-capturing of the reservoir fines may give rise to reduction of the permeability in water swept zones, which subsequently leads to the diversion of water flow from the initially more permeable layers to the less permeable ones. As a result, the displacement is more even, the water cut at the producer is decreased, and the oil recovery is increased. On the other hand, more energy for the pressure drop is required to maintain a constant flow rate. These effects are studied within a new upscaling model developed previously (Zhang et al., 2011). In a communicating layer cake reservoir, higher end-point mobility ratio (water to oil) leads to more crossflow between layers and lowers the water sweep efficiency. However, this ratio facilitates the fluid diversion caused by the fines migration, leading to a more efficient enhanced oil recovery. The positive contribution from the mobility ratio to the increased oil recovery due to fines migration seems to be limited.

General information
State: Published
Organisations: CERE – Center for Energy Ressources Engineering, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Yuan, H. (Intern), Shapiro, A. (Intern)
Pages: 618-626
Publication date: 2011
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Petroleum Science and Engineering
Volume: 78
Issue number: 3-4
ISSN (Print): 0920-4105
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.56 SJR 0.764 SNIP 1.631
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.801 SNIP 1.652 CiteScore 2.38
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.692 SNIP 1.751 CiteScore 1.95
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.822 SNIP 1.901 CiteScore 1.73
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.774 SNIP 1.666 CiteScore 1.42
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.648 SNIP 1.41 CiteScore 1.29
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.746 SNIP 1.724
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.072 SNIP 1.852
Upscaling of Two-Phase Immiscible Flows in Communicating Stratified Reservoirs

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

General information
State: Published
Organisations: CERE – Center for Energy Ressources Engineering, Department of Chemical and Biochemical Engineering, Department of Chemistry
Authors: Niu, B. (Intern), Shapiro, A. (Intern), Yan, W. (Intern), Stenby, E. H. (Intern)
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Publisher: Technical University of Denmark (DTU)
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Original language: English
Main Research Area: Technical/natural sciences
Electronic versions:
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Source: orbit
Source-ID: 264503
Publication: Research - peer-review › Journal article – Annual report year: 2011

1D Simulations for Microbial Enhanced Oil Recovery with Metabolite Partitioning
We have developed a mathematical model describing the process of microbial enhanced oil recovery (MEOR). The one-dimensional isothermal model comprises displacement of oil by water containing bacteria and substrate for their feeding. The bacterial products are both bacteria and metabolites. In the context of MEOR modeling, a novel approach is partitioning of metabolites between the oil and the water phases. The partitioning is determined by a distribution coefficient. The transfer part of the metabolite to oil phase is equivalent to its “disappearance”, so that the total effect from of metabolite in the water phase is reduced. The metabolite produced is surfactant reducing oil–water interfacial tension, which results in oil mobilization. The reduction of interfacial tension is implemented through relative permeability curve
modifications primarily by lowering residual oil saturation. The characteristics for the water phase saturation profiles and the oil recovery curves are elucidated. However, the effect from the surfactant is not necessarily restricted to influence only interfacial tension, but it can also be an approach for changing, e.g., wettability. The distribution coefficient determines the time lag, until residual oil mobilization is initialized. It has also been found that the final recovery depends on the distance from the inlet before the surfactant effect takes place. The surfactant effect position is sensitive to changes in maximum growth rate, and injection concentrations of bacteria and substrate, thus determining the final recovery.

Different methods for incorporating surfactant-induced reduction of interfacial tension into models are investigated. We have suggested one method, where several parameters can be estimated in order to obtain a better fit with experimental data. For all the methods, the incremental recovery is very similar, only coming from small differences in water phase saturation profiles. Overall, a significant incremental oil recovery can be achieved, when the sensitive parameters in the context of MEOR are carefully dealt with.

**General information**

State: Published
Organisations: CERE – Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Nielsen, S. M. (Intern), Shapiro, A. (Intern), Michelsen, M. L. (Intern), Stenby, E. H. (Intern)
Pages: 785-802
Publication date: 2010
Main Research Area: Technical/natural sciences

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BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.16 SJR 0.767 SNIP 1.316
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.728 SNIP 1.317 CiteScore 1.94
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.932 SNIP 1.433 CiteScore 1.91
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.04 SNIP 1.433 CiteScore 2.03
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.942 SNIP 1.522 CiteScore 1.88
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.921 SNIP 1.337 CiteScore 1.81
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.615 SNIP 1.203
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.612 SNIP 1.088
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Advanced Waterflooding in Carbonate Reservoirs

General information
State: Published
Organisations: CERE – Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering
Authors: Zahid, A. (Intern), Stenby, E. H. (Intern), Shapiro, A. (Intern)
Publication date: 2010
Event: Poster session presented at 11th International Symposium on Evaluation of Wettability and Its Effect on Oil Recovery, University of Calgary, Alberta, Canada.
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 258646
Publication: Research - peer-review › Journal article – Annual report year: 2010

A Stochastic Theory for Deep Bed Filtration Accounting for Dispersion and Size Distributions

We develop a stochastic theory for filtration of suspensions in porous media. The theory takes into account particle and pore size distributions, as well as the random character of the particle motion, which is described in the framework of the theory of continuous-time random walks (CTRW). In the limit of the infinitely many small walk steps we derive a system of governing equations for the evolution of the particle and pore size distributions. We consider the case of concentrated suspensions, where plugging the pores by particles may change porosity and other parameters of the porous medium. A procedure for averaging of the derived system of equations is developed for polydisperse suspensions with several distinctive particle sizes. A numerical method for solution of the flow equations is proposed. Sample calculations are applied to compare the roles of the particle size distribution and of the particle flight dispersion on the deposition profiles. It is demonstrated that the temporal flight dispersion is the most likely mechanism forming the experimentally observed hyperexponential character of the deposition profiles.

General information
State: Published
Organisations: CERE – Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Shapiro, A. (Intern), Bedrikovetsky, P. G. (Ekstern)
Pages: 2473-2494
Publication date: 2010
Main Research Area: Technical/natural sciences

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Volume: 389
Issue number: 13
ISSN (Print): 0378-4371
Ratings:
Improved Oil Recovery in Chalk: Wettability Alteration or Something Else?

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering
Improved Oil Recovery in Chalk: Wettability Alteration or Something Else?

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

Publication information
Journal: SPE Journal
Volume: 131
ISSN (Print): 1086-055X
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.01 SJR 0.95 SNIP 2.003
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.976 SNIP 1.838 CiteScore 2.37
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.185 SNIP 2.152 CiteScore 2.43
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.993 SNIP 1.773 CiteScore 2.25
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.047 SNIP 1.757 CiteScore 2.13
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.139 SNIP 1.757 CiteScore 2.3
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.143 SNIP 2.103
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.106 SNIP 1.642
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.513 SNIP 1.369
Scopus rating (2007): SJR 0.677 SNIP 0.894
Scopus rating (2006): SJR 1.09 SNIP 1.93
Web of Science (2006): Indexed yes
In-Situ Phase Identification and Saturation Determination in Carbon Dioxide Flooding of Water Flooded Chalk Using X-Ray Computed Tomography

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering
Authors: Niu, B. (Intern), Yan, W. (Intern), Shapiro, A. (Intern), Stenby, E. H. (Intern)
Pages: 129760
Publication date: 2010
Main Research Area: Technical/natural sciences

Publication information
Journal: S P E Journal
ISSN (Print): 1086-055X
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.01 SJR 0.95 SNIP 2.003
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.976 SNIP 1.838 CiteScore 2.37
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.185 SNIP 2.152 CiteScore 2.43
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.993 SNIP 1.773 CiteScore 2.25
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.047 SNIP 1.757 CiteScore 2.13
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.139 SNIP 1.757 CiteScore 2.3
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.143 SNIP 2.103
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
In-Situ Phase Identification and Saturation Determination in Carbon Dioxide Flooding of Water Flooding Chalk Using X-Ray Computed Tomography

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering
Authors: Niu, B. (Intern), Yan, W. (Intern), Shapiro, A. (Intern), Stenby, E. H. (Intern)
Number of pages: 13
Publication date: 2010

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Publisher: Society of Petroleum Engineers
Main Research Area: Technical/natural sciences
Conference: SPE Improved Oil Recovery Symposium, Oklahoma, USA, 01/01/2010
DOIs: 10.2118/129760-MS
Source: orbit
Source-ID: 264500
Publication: Research - peer-review › Article in proceedings – Annual report year: 2010

Microbial Enhanced Oil Recovery: 3D Simulation with Gravity Effects
Microbial enhanced oil recovery (MEOR) utilizes the activity of microorganisms, where microorganisms simultaneously grow in a reservoir and convert substrate into recovery enhancing products (usually, surfactants). In order to predict the performance of a MEOR process, a simulation tool is required, with all the relevant physical processes included.

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

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

We investigate the benefit of MEOR relative to water flooding, comparing the processes in multiple dimensions.

The results of our simulations demonstrate that the oil recovery from MEOR processes in relation to water flooding is
markedly increased, and the high recovery is achieved much faster. In addition, the compositional streamline simulator is applied to study both microscopic and macroscopic displacement efficiency of MEOR.

**General information**
State: Published
Organisations: CERE – Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering
Authors: Nielsen, S. M. (Intern), Jessen, K. (Ekstern), Shapiro, A. (Intern), Michelsen, M. L. (Intern), Stenby, E. H. (Intern)
Number of pages: 11
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ISBN (Print): 978-90-73781-86-3
Series: SPE 131048
Main Research Area: Technical/natural sciences
Conference: SPE EUROPEC/EAGE Annual Conference and Exhibition, Barcelona, Spain, 14/06/2010 - 14/06/2010
DOIs: 10.2118/131048-MS
Source: orbit
Source-ID: 266998
Publication: Research - peer-review › Article in proceedings – Annual report year: 2010

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

General information
State: Published
Organisations: CERE – Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, Department of Chemistry
Authors: Nielsen, S. M. (Intern), Shapiro, A. (Intern), Stenby, E. H. (Intern), Michelsen, M. L. (Intern)
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Electronic versions:
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Source: orbit
Source-ID: 274917
Publication: Research › Ph.D. thesis – Annual report year: 2010

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

General information
State: Published
Organisations: CERE – Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering
Authors: Yuan, H. (Intern), Shapiro, A. (Intern)
Pages: 974-988
Publication date: 2010
Main Research Area: Technical/natural sciences

Publication information
Journal: Chemical Engineering Journal
Volume: 162
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Ratings:
Tertiary Carbon Dioxide Flooding of Low Permeable Chalk with In-Situ Saturation Determination using X-Ray Computed Tomography

General information
State: Published
Organisations: CERE – Center for Energy Ressources Engineering, Department of Chemical and Biochemical Engineering
Authors: Niu, B. (Intern), Yan, W. (Intern), Shapiro, A. (Intern), Stenby, E. H. (Intern)
Publication date: 2010
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 264504
Publication: Research - peer-review › Journal article – Annual report year: 2010

DOI: 10.1016/j.cej.2010.07.003
Source: orbit
Source-ID: 274762
Publication: Research - peer-review › Poster – Annual report year: 2010
Transport of reservoir fines: a novel model for formation heterogeneity and particle heterogeneity

Modeling transport of reservoir fines is of great importance for evaluating the damage of production wells and infectivity decline. The conventional methodology accounts for neither the formation heterogeneity around the wells nor the reservoir fines' heterogeneity. We have developed an integral model incorporating the elliptic equation based on continuous time random walk and distributed filtration coefficients, respectively reflecting the influences of the formation heterogeneity around the wells and the reservoir fines' heterogeneity. The novel methodology excels the classical advection dispersion equation in modeling the transport and the deposition of reservoir fines. It successfully predicts the unsymmetrical concentration profiles and the hyperexponential deposition in experiments.

A New Approach to Modeling Immiscible Two-phase Flow in Porous Media

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

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
Title of host publication: Proceeding in CD from European COMSOL Conference
Mathematical Model for Microbial Enhanced Oil Recovery with Surfactant Distributed between Phases

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

Modeling adsorption of liquid mixtures on porous materials

The multicomponent potential theory of adsorption (MPTA), which was previously applied to adsorption from gases, is extended onto adsorption of liquid mixtures on porous materials. In the MPTA, the adsorbed fluid is considered as an inhomogeneous liquid with thermodynamic properties that depend on the distance from the solid surface (or position in the porous space). The theory describes the two kinds of interactions present in the adsorbed fluid, i.e. the fluid-fluid and fluid-solid interactions, by means of an equation of state and interaction potentials, respectively. The proposed extension of the MPTA onto liquids has been tested on experimental binary and ternary adsorption data. We show that, for the set of experimental data considered in this work, the MPTA model is capable of correlating binary adsorption equilibria. Based on binary adsorption data, the theory can then predict ternary adsorption equilibria. Good agreement with the theoretical predictions is achieved in most of the cases. Some limitations of the model are also discussed.

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Monsalvo, M. A. (Intern), Shapiro, A. (Intern)
Pages: 310-316
Publication date: 2009
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Colloid and Interface Science
Volume: 333
Issue number: 1
ISSN (Print): 0021-9797
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 4.14 SJR 1.144 SNIP 1.267
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.095 SNIP 1.263 CiteScore 3.8
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.166 SNIP 1.406 CiteScore 3.74
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
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

Study of high-pressure adsorption from supercritical fluids by the potential theory
The multicomponent potential theory of adsorption (MPTA), which has been previously used to study low-pressure adsorption of subcritical fluids, is extended to adsorption equilibria from supercritical fluids up to high pressures. The MPTA describes an adsorbed phase as an inhomogeneous fluid with thermodynamic properties that depend on the distance from the solid surface (or position in the porous space). The description involves the two kinds of interactions present in the adsorbed fluid, i.e. the fluid-fluid and fluid-solid interactions. accounted for by means of an equation of state (EoS) and interaction potential functions, respectively. This makes it possible to generate the different MPTA models by combination of the relevant EoS/potentials. In the present work, the simplified perturbed-chain statistical associating fluid theory (sPC-SAFT) EoS is used for the thermodynamic description of both the adsorbed and the gas phases. We have also evaluated the performance of the classical Soave-Redlich-Kwong (SRK) EoS. The fluid-solid interactions are described by simple Dubinin-Radushkevich-Astakhov (DRA) potentials. In addition, we test the performance of the 10-4-3 Steele potential. It is shown that application of sPC-SAFT slightly improves the performance of the MPTA and that in spite of its simplicity, the DRA model can be considered as an accurate potential, especially, for mixture adsorption. We show that, for the sets of experimental data considered in this work, the MPTA is capable of predicting adsorption of pure components and binary mixtures in wide ranges of pressure and temperature. A good agreement with the theoretical predictions is achieved in most of the cases. The MPTA is capable to correctly describe complex physical behavior observed at supercritical/high-pressure conditions. Some limitations of the model are also discussed.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Phase Equilibria and Separation Processes, Center for Energy Resources Engineering
Authors: Monsalvo, M. A. (Intern), Shapiro, A. (Intern)
Pages: 56-64
Publication date: 2009
Main Research Area: Technical/natural sciences

Publication information
Journal: Fluid Phase Equilibria
Volume: 283
Issue number: 1-2
ISSN (Print): 0378-3812
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
Statistical methods for history matching


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

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

Behavior of Fluid Mixtures in Porous Materials

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering
Authors: Monsalvo, M. A. (Intern), Shapiro, A. (Intern)
Publication date: 2008
Event: Poster session presented at SPE Meeting, Hellerup, Denmark.
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 232054
Publication: Research › Poster – Annual report year: 2008

Elliptic random-walk equation for suspension and tracer transport in porous media

We propose a new approach to transport of the suspensions and tracers in porous media. The approach is based on a modified version of the continuous time random walk (CTRW) theory. In the framework of this theory we derive an elliptic transport equation. The new equation contains the time and the mixed dispersion terms expressing the dispersion of the particle time steps. The properties of the new equation are studied and the fundamental analytical solutions are obtained. The solution of the pulse injection problem describing a common tracer injection experiment is studied in greater detail. The new theory predicts delay of the maximum of the tracer, compared to the velocity of the flow, while its forward "tail" contains much more particles than in the solution of the classical parabolic (advection-dispersion) equation. This is in agreement with the experimental observations and predictions of the CTRW theory. (C) 2008 Elsevier B.V. All rights reserved.
Fractional Flow Model for Suspension Transport in Porous Media

**General information**
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Bedrikovetsky, P. (Ekstern), Shapiro, A. (Intern)
Publication date: 2008

**Host publication information**
Title of host publication: 10th World Filtration Congress
Main Research Area: Technical/natural sciences
Conference: World Filtration Congress, Leipzig, Germany, 01/01/2008
Source: orbit
Source-ID: 219858
Publication: Research - peer-review › Article in proceedings – Annual report year: 2008

Gas transport in tight porous media

Gas kinetic approach
We describe the flow of gas in a porous medium in the kinetic regime, where the viscous flow structure is not formed in separate pores. Special attention is paid to the dense kinetic regime, where the interactions within the gas are as important as the interaction with the porous medium. The transport law for this regime is derived by means of the gas kinetic theory, in the framework of the model of "heavy gas in light one". The computations of the gas kinetic theory are confirmed by the dimension analysis and a simplified derivation revealing the considerations behind the kinetic derivation. The role of the thermal gradient in the transport law is clarified. (c) 2007 Elsevier B.V. All rights reserved.

**General information**
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Shapiro, A. (Intern), Wesselingh, J. (Intern)
Pages: 14-22
Publication date: 2008
Main Research Area: Technical/natural sciences

**Publication information**
Journal: Chemical Engineering Journal
Volume: 142
Issue number: 1
ISSN (Print): 1385-8947
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 6.34
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 5.68
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 4.92
Phase Behavior in Confined Systems

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering
Authors: Monsalvo, M. A. (Intern), Shapiro, A. (Intern)
Publication date: 2008
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 232092
Publication: Research › Poster – Annual report year: 2008

Random-Walk Description of Suspension Transport in Porous Media

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Bedrikovetsky, P. (Ekstern), Shapiro, A. (Intern)
Publication date: 2008

Host publication information
Title of host publication: ICTAM 2008
Main Research Area: Technical/natural sciences
Source: orbit
A stochastic model for filtration of particulate suspensions with incomplete pore plugging

A population balance model for particulate suspension transport with capture of particles by porous medium accounting for complete and incomplete plugging of pores by retained particles is derived. The model accounts for pore space accessibility, due to restriction on finite size particle movement through the overall pore space, and for particle flux reduction, due to transport of particles by the fraction of the overall flux. The novel feature of the model is the residual pore conductivity after the particle retention in the pore and the possibility of one pore to capture several particles. A closed system of governing stochastic equations determines the evolution of size distributions for suspended particles and pores. Its averaging results in the closed system of hydrodynamic equations accounting for permeability and porosity reduction due to plugging. The problem of deep bed filtration of a single particle size suspension through a single pore size medium where a pore can be completely plugged by two particles allows for an exact analytical solution. The phenomenological deep bed filtration model follows from the analytical solution.
Scopus rating (2009): SJR 0.612 SNIP 1.088
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.7 SNIP 0.924
Scopus rating (2007): SJR 0.717 SNIP 1.215
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 0.929 SNIP 1.284
Scopus rating (2005): SJR 0.918 SNIP 1.293
Scopus rating (2004): SJR 1.071 SNIP 1.227
Scopus rating (2003): SJR 0.879 SNIP 1.195
Scopus rating (2002): SJR 0.982 SNIP 0.938
Scopus rating (2001): SJR 1.006 SNIP 0.975
Scopus rating (2000): SJR 0.896 SNIP 0.732
Web of Science (2000): Indexed yes
Scopus rating (1999): SJR 0.571 SNIP 1.065
Original language: English
Links:
http://www.springerlink.com/content/u41241x7651177w6/
Source: orbit
Source-ID: 189552
Publication: Research - peer-review › Journal article – Annual report year: 2007

**Diffusion measurements in binary liquid mixtures by Raman spectroscopy**

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

**General information**

State: Published
Organisations: Energy and Materials, Department of Chemistry, Department of Chemical and Biochemical Engineering, Center for Phase Equilibria and Separation Processes, Center for Energy Resources Engineering
Authors: Berg, R. W. (Intern), Hansen, S. B. (Intern), Shapiro, A. (Intern), Stenby, E. H. (Intern)
Pages: 367-373
Publication date: 2007
Main Research Area: Technical/natural sciences

**Publication information**

Journal: Applied Spectroscopy
Volume: 61
Issue number: 4
ISSN (Print): 0003-7028
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 0.48 SNIP 0.967 CiteScore 1.76
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Diffusionsmålinger med Ramanspektroskopi: Viden om diffusioner er i mange sammenhænge af stor betydning. Her beskrives en simpel måde til at studere diffusioner i væsker

General information
State: Published
Organisations: Department of Chemistry, Energy and Materials, Department of Chemistry, Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering
Authors: Hansen, S. B. (Intern), Berg, R. W. (Intern), Shapiro, A. (Intern), Stenby, E. H. (Intern)
Elliptic equation for random walks. Application to transport in microporous media

We consider a process of random walks with arbitrary residence time distribution. We show that in many cases this process may not be described by the classical (Fick) parabolic diffusion equation, but an elliptic equation. An additional term proportional to the second time derivative takes into account the distribution of the residence times of molecules ill pores. The new elliptic diffusion equation is strictly derived by the operator approach. A criterion showing where the new equation should be applied instead of the standard diffusion equation is obtained. Boundary conditions are studied and a principle for selection of a unique bounded solution is formulated. Fundamental solutions are obtained and compared with the results of direct simulation of the random walks. (c) 2006 Elsevier B.V. All rights reserved.
Modeling adsorption of binary and ternary mixtures on microporous media

The goal of this work is to analyze the adsorption of binary and ternary mixtures on the basis of the multicomponent potential theory of adsorption (MPTA). In the MPTA, the adsorbate is considered as a segregated mixture in the external potential field emitted by the solid adsorbent. This makes it possible using the same equation of state to describe the thermodynamic properties of the segregated and the bulk phases. For comparison, we also used the ideal adsorbed solution theory (IAST) to describe adsorption equilibria. The main advantage of these two models is their capabilities to predict multicomponent adsorption equilibria on the basis of single-component adsorption data. We compare the MPTA and IAST models to a large set of experimental data, obtaining reasonable good agreement with experimental data and high degree of predictability. Some limitations of both models are also discussed.

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Monsalvo, M. A. (Intern), Shapiro, A. (Intern)
Pages: 91-100
Publication date: 2007
Main Research Area: Technical/natural sciences

Publication information
Journal: Fluid Phase Equilibria
Volume: 254
Issue number: 1-2
ISSN (Print): 0378-3812
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 2.33 SJR 0.869 SNIP 1.155
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.874 SNIP 0.998 CiteScore 1.99
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 0.982 SNIP 1.248 CiteScore 2.28
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.007 SNIP 1.274 CiteScore 2.31
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.152 SNIP 1.286 CiteScore 2.31
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.034 SNIP 1.234 CiteScore 2.26
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 0.986 SNIP 1.317
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.133 SNIP 1.164
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.227 SNIP 1.09
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.031 SNIP 1.151
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.034 SNIP 1.245
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.009 SNIP 1.3
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 0.985 SNIP 1.349
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 1.193 SNIP 1.301
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 0.722 SNIP 1.101
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 0.966 SNIP 1.284
Prediction of adsorption from liquid mixtures in microporous media by the potential theory

Despite its industrial importance, adsorption from the liquid phase has been studied much less extensively than adsorption from the gas phase. In this paper, we study the adsorption of liquid mixtures on the basis of the multicomponent potential theory of adsorption (MPTA). The MPTA is based on the potential concept originally developed by Polanyi. In this theory, the driving force for physical adsorption is measured by the adsorption potential that is a function of the distance from the solid surface. In this way, the adsorbate is considered as a heterogeneous substance segregated in the external field emitted by the adsorbent, with thermodynamic parameters that are function of the distance from the solid. The MPTA then uses a thermodynamic model to describe the equilibrium between bulk and adsorbed phases (or the fluid-fluid interactions), and potential models for the fluid-solid interactions. With this approach, few parameters are needed to predict adsorption equilibria. The MPTA has been so far used to successfully predict adsorption equilibria of multicomponent gas mixtures. The aim of this work is to extent the MPTA onto adsorption from liquid solutions. We show that such extension is straightforward, obtaining relatively simple models useful for engineering applications. Comparison with experimental data shows good agreement and high degree of predictability. (C) 2007 Elsevier B.V. All rights reserved.
Phase Behavior and Viscosity Modeling of Refrigerant-Lubricant Mixtures

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Phase Equilibria and Separation Processes
Authors: Monsalvo, M. A. (Intern), Shapiro, A. (Intern), Thomsen, K. (Intern)
Publication date: Mar 2006

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Electronic versions:
Matia A Monsalvo.pdf
Source: orbit
Source-ID: 241289
Publication: Research › Ph.D. thesis – Annual report year: 2006

Adsorption of Multicomponent Mixtures on Heterogeneous Microporous Solids

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering
Authors: Monsalvo, M. A. (Intern), Shapiro, A. (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: 192806
Publication: Research - peer-review › Poster – Annual report year: 2006

A splitting technique for analytical modelling of two-phase multicomponent flow in porous media
In this paper we discuss one-dimensional models for two-phase Enhanced Oil Recovery (EOR) floods (oil displacement by gases, polymers, carbonized water, hot water, etc.). The main result presented here is the splitting of the EOR mathematical model into thermodynamical and hydrodynamical parts. The introduction of a potential associated with one of the conservation laws and its use as a new independent coordinate reduces the number of equations by one. The (n)x(n) conservation law model for two-phase n-component EOR flows in new coordinates is transformed into a reduced (n-1)x(n-1) auxiliary system containing just thermodynamical variables (equilibrium fractions of components, sorption isotherms) and one lifting equation containing just hydrodynamical parameters (phase relative permeabilities and viscosities). The algorithm to solve analytically the problem includes solution of the reduced auxiliary problem, solution of one lifting hyperbolic equation and inversion of the coordinate transformation. The splitting allows proving the independence of phase transitions occurring during displacement of phase relative permeabilities and viscosities. For example, the minimum miscibility pressure (MMP) and transitional tie lines are independent of relative permeabilities and phases viscosities. Relative motion of polymer, surfactant and fresh water slugs depends on sorption isotherms only. Therefore, MMP for gasflood or minimum fresh water slug size providing isolation of polymer/surfactant from incompatible formation water for chemical flooding can be calculated from the reduced auxiliary system. Reduction of the number of equations allows the generation of new analytical models for EOR. The analytical model for displacement of oil by a polymer slug with water drive is presented.

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Dissolution of Light Hydrocarbons in Drilling Muds, Prediction of the Nature of Reservoir Fluids Based on Gas Shows

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering
Authors: Liège, X. C. (Ekstern), Shapiro, A. (Intern)
Publication date: 2006

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Electronic versions:
Xavier Liege, ph.d..pdf
Source: orbit
Source-ID: 199159
Publication: Research › Journal article – Annual report year: 2006

Experimental investigation of the diffusion coefficients in porous media by application of X-ray computer tomography
The present work describes a new experimental method that makes it possible to investigate diffusion coefficients in a porous medium. The method is based on application of X-ray computed tomography (CT). The general applicability of this method for the determination of diffusion coefficients is demonstrated. A series of such experiments was carried out. Several samples of carbonaceous and sandstone rock were investigated. The diffusion coefficients in porous media were determined by measuring the concentration of salt in different slices of a sample as a function of time. In cases where stable values of diffusion coefficients were obtained (all samples except for one highly heterogeneous sample), these values served for the determination of the tortuosity-porosity factors for a given type of porous medium.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Phase Equilibria and Separation Processes, Center for Energy Resources Engineering
Authors: Zhelezny, P. (Intern), Shapiro, A. (Intern)
Pages: 275-288
Publication date: 2006
Main Research Area: Technical/natural sciences

Publication Information
Journal: Journal of Porous Media
Volume: 9
Issue number: 4
ISSN (Print): 1091-028X
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 0.492 SNIP 0.744 CiteScore 1.22
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.456 SNIP 0.789 CiteScore 1.05
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.365 SNIP 0.654 CiteScore 0.81
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.295 SNIP 0.488 CiteScore 0.6
Modeling Phase Equilibria and Volumetric Behavior of Refrigerant + Lubricant Mixtures

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering
Authors: Monsalvo, M. A. (Intern), Shapiro, A. (Intern), Thomsen, K. (Intern)
Publication date: 2006
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 199162
Publication: Research - peer-review › Journal article – Annual report year: 2006

Multicomponent Adsorption Approaches to Modeling Adsorption Equilibria

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

Host publication information
Title of host publication: Encyclopedia of Surface and Colloid Science
Place of publication: New York
Publisher: C R C Press LLC
Edition: Second
ISBN (Print): 9780849396151
On the Process of Gas Liberation in Porous Media

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

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Phase Equilibria and Separation Processes, Center for Energy Resources Engineering
Authors: Zhelezny, P. (Intern), Shapiro, A. (Intern), Vu, D. T. (Intern), Stenby, E. H. (Intern)
Pages: 503-521
Publication date: 2006
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Porous Media
Volume: 9
Issue number: 6
ISSN (Print): 1091-028X
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 0.492 SNIP 0.744 CiteScore 1.22
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.456 SNIP 0.789 CiteScore 1.05
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.365 SNIP 0.654 CiteScore 0.81
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.295 SNIP 0.488 CiteScore 0.6
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.385 SNIP 0.617 CiteScore 0.65
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.388 SNIP 0.943 CiteScore 0.81
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.411 SNIP 0.689
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.323 SNIP 0.621
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.472 SNIP 0.509
Scopus rating (2007): SJR 0.322 SNIP 0.623
Scopus rating (2006): SJR 0.671 SNIP 0.653
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.07 SNIP 1.4
**Statistical Methods for History Matching**

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**General information**

State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering
Authors: Johansen, K. (Intern), Shapiro, A. (Intern), Stenby, E. H. (Intern)
Publication date: 2006
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 199161
Publication: Research - peer-review › Journal article – Annual report year: 2003

**Diffusion Coefficients in Multicomponent Mixtures**

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**General information**

State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Phase Equilibria and Separation Processes
Authors: Medvedev, O. (Intern), Shapiro, A. (Intern)
Publication date: 2005

**Publication information**

Original language: English
Main Research Area: Technical/natural sciences
Electronic versions:
Oleg Medvedev, ph.d..pdf
Source: orbit
Source-ID: 193453
Publication: Research - peer-review › Poster – Annual report year: 2006

**Modeling diffusion coefficients in binary mixtures of polar and non-polar compounds**

The theory of transport coefficients in liquids, developed previously, is tested on a description of the diffusion coefficients in binary polar/non-polar mixtures, by applying advanced thermodynamic models. Comparison to a large set of experimental data shows good performance of the model. Only four temperature-independent parameters are required in order to describe the behavior of diffusion coefficients at different temperatures. The physical meaning of the parameters is analyzed. This makes it possible to reduce further their number to just two parameters for described mixtures with polar components and to only one parameter for mixtures consisting of non-polar components. A possibility of complete prediction of the parameters is discussed.

**General information**

State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Phase Equilibria and Separation Processes, Center for Energy Resources Engineering
Authors: Medvedev, O. (Intern), Shapiro, A. (Intern)
Pages: 111-124
Publication date: 2005
Main Research Area: Technical/natural sciences

**Publication information**
Molecular dynamics simulations of the penetration lengths: application within the fluctuation theory for diffusion coefficients

Mutual diffusion in condensed phases is a theoretically and practically important subject of active research. One of the most rigorous and theoretically advanced approaches to the problem is a recently developed approach based on the concept of penetration lengths (Physica A 320 (2003) 211; Physica A 322 (2004) 151). In the current study, a fast molecular dynamics scheme has been developed to determine the values of the penetration lengths in Lennard-Jones binary systems. Results deduced from computations provide a new insight into the concept of penetration lengths. It is shown for four different binary liquid mixtures of non-polar components that computed penetration lengths, for various temperatures and compositions, are consistent with those deduced from experiments in the framework of the formalism of the fluctuation theory. Moreover, the mutual diffusion coefficients obtained from a coupled fluctuation theory and molecular dynamics scheme exhibit consistent trends and average deviations from experimental data around 10-20%. (c) 2004 Elsevier B.V. All rights reserved.
Modeling the Thermal Diffusion Coefficients

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Phase Equilibria and Separation Processes
Authors: Gonzales Bagnoli, M. G. (Intern), Shapiro, A. (Intern)
Publication date: Dec 2004

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Electronic versions:
Marina Gabriela, ph.d..pdf
Source: orbit
Source-ID: 185082
Publication: Research - peer-review › Journal article – Annual report year: 2005

Analytical Model for 1-D Gas Flooding: Splitting between Hydrodynamics and Thermodynamics

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Pires, A. (Ekstern), Bedrikovetsky, P. G. (Ekstern), Shapiro, A. (Intern)
Pages: 6
Publication date: 2004
Main Research Area: Technical/natural sciences

Publication information
Journal: SPE/DOE Symposium on Improved Oil Recovery
Volume: 0
Issue number: 0
Diffusion measurements by Raman spectroscopy

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

Fluctuation theory for transport properties in multicomponent mixtures: thermodiffusion and heat conductivity
The theory of transport properties in multicomponent gas and liquid mixtures, which was previously developed for diffusion coefficients, is extended onto thermodiffusion coefficients and heat conductivities. The derivation of the expressions for transport properties is based on the general statistical theory of fluctuations around an equilibrium state. The Onsager matrix of phenomenological coefficients is expressed in terms of the penetration lengths, including the newly introduced penetration length for the energy transfer. As an example, this penetration length is found from the known value of the heat conductivity coefficient for ideal gas. (C) 2003 Elsevier B.V. All rights reserved.
Modeling Diffusion Coefficients in Binary Mixtures

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Medvedev, O. (Intern), Shapiro, A. (Intern)
Pages: 13-22
Publication date: 2004
Main Research Area: Technical/natural sciences

Publication information
Journal: Fluid Phase Equilibria
Volume: 225
Issue number: 0
ISSN (Print): 0378-3812
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 2.33 SJR 0.869 SNIP 1.155
Streamline Simulation with Capillary Effects Applied to Petroleum Engineering Problems

General information
State: Published
Three-phase Compositional Streamline Simulation and Its Application to WAG

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Yan, W. (Intern), Michelsen, M. L. (Intern), Stenby, E. H. (Intern), Berenblyum, R. (Intern), Shapiro, A. (Intern)
Number of pages: 11
Publication date: 2004
Main Research Area: Technical/natural sciences
DOIs:
10.2118/89440-MS
Source: orbit
Source-ID: 262146
Publication: Research - peer-review › Paper – Annual report year: 2004

Black Oil Streamline Simulator with Capillary Effects

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

Bibliographical note
Pub.internno: SEP0316
converted by kit2ddf.pl 1.01
WWW: cataloguer/id is not the CWIS of the main author
Source: orbit
Source-ID: 41367
Publication: Research › Poster – Annual report year: 2003

Black Oil Streamline Simulator with Capillary Effects

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

Host publication information
Title of host publication: Proceedings of the Annual workshop of the IEA Collaborative Project on Enhanced Oil Recovery Agreement
Main Research Area: Technical/natural sciences
Compositional Streamline Simulation: Progress Report No. 4

Evaluation of diffusion coefficients in multicomponent mixtures by means of the fluctuation theory

We derive general expressions for diffusion coefficients in multicomponent non-ideal gas or liquid mixtures. The derivation is based on the general statistical theory of fluctuations around an equilibrium state. The matrix of diffusion coefficients is expressed in terms of the equilibrium thermodynamic characteristics of the mixture (such as molar densities and internal energy), as well as in terms of the newly introduced parameters, the penetration lengths. This result serves to reduce the problem of determining the diffusion coefficients to a smaller number of physically meaningful characteristics. We demonstrate on several examples that the developed theory is in agreement with the established experimental facts and dependencies for the diffusion coefficients. (C) 2002 Elsevier Science B.V. All rights reserved.
Evaluation of the Thermodynamic Models for the Thermal Diffusion Factor

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

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

Publication information
Journal: Philosophical Magazine
Volume: 83
ISSN (Print): 1478-6435
Ratings:
BFI (2018): BFI-level 1
Verifying reciprocal relations for experimental diffusion coefficients in multicomponent mixtures

The goal of the present study is to verify the agreement of the available data on diffusion in ternary mixtures with the theoretical requirement of linear non-equilibrium thermodynamics consisting in symmetry of the matrix of the phenomenological coefficients. A common set of measured diffusion coefficients for a three-component mixture consists of four Fickian diffusion coefficients, each being reported separately. However, the Onsager theory predicts the existence of only three independent coefficients, as one of them disappears due to the symmetry requirement. Re-calculation of the Fickian diffusion coefficients into Onsager coefficients for a non-ideal mixture involves derivatives of the chemical potentials and, thus, should be based on a certain thermodynamic model (cubic equation of state (EoS), an activity coefficient model, etc.). Transformation of the Fickian diffusion coefficients into Onsager coefficients and a subsequent
symmetry check make it possible to evaluate different thermodynamic models with regard to their possibility of being used for prediction of the transport properties. We performed several checks of this kind for ternary mixtures of hydrocarbons and alcohols, where extended sets of experimental data and reliable thermodynamic models were available. The sensitivity of the symmetry property to different thermodynamic parameters of the models was also checked. (C) 2003 Elsevier Science B.V. All rights reserved.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering, Center for Energy Resources Engineering
Authors: Medvedev, O. (Intern), Shapiro, A. (Intern)
Pages: 291-301
Publication date: 2003
Main Research Area: Technical/natural sciences

Publication information
Journal: Fluid Phase Equilibria
Volume: 208
Issue number: 1-2
ISSN (Print): 0378-3812
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 2.33 SJR 0.869 SNIP 1.155
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.874 SNIP 0.998 CiteScore 1.99
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 0.982 SNIP 1.248 CiteScore 2.28
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.007 SNIP 1.274 CiteScore 2.31
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.152 SNIP 1.286 CiteScore 2.31
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.034 SNIP 1.234 CiteScore 2.26
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 0.986 SNIP 1.317
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.133 SNIP 1.164
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.227 SNIP 1.09
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.031 SNIP 1.151
Web of Science (2007): Indexed yes
Diffusion in Multicomponent Mixtures

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Shapiro, A. (Intern), Davis, P. K. (Ekstern), Duda, J. L. (Ekstern)
Publication date: 2002

Host publication information
Title of host publication: Computer Aided Property Estimation
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 209314
Publication: Research - peer-review › Book chapter – Annual report year: 2002

Effect of Geothermal Gradients on Fluid Distribution in Petroleum 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: Shapiro, A. (Intern), Stenby, E. H. (Intern)
Publication date: 2002

Host publication information
Title of host publication: Encyclopedia of Petroleum Engineering
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 209313
Publication: Research - peer-review › Book chapter – Annual report year: 2002

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

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

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Shapiro, A. (Intern), Stenby, E. H. (Intern)
Pages: 61-73
Publication date: 2002
Main Research Area: Technical/natural sciences
Publication information
Journal: Lecture Notes in Physics
Volume: 584
ISSN (Print): 1616-6361
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 0.591 SNIP 0.382 CiteScore 0.55
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.661 SNIP 0.428 CiteScore 0.8
Thermodynamics of the multicomponent vapor-liquid equilibrium under capillary pressure difference

We discuss the two-phase multicomponent equilibrium, provided that the phase pressures are different due to the action of capillary forces. We prove the two general properties of such an equilibrium, which have previously been known for a single-component case, however, to the best of our knowledge, not for the multicomponent mixtures. The importance is emphasized on the space of the intensive variables \( P, T \) and \( \mu_i \), where the laws of capillary equilibrium have a simple geometrical interpretation. We formulate thermodynamic problems specific to such an equilibrium, and outline changes to be introduced to common algorithms of flash calculations in order to solve these problems. Sample calculations show large variation of the capillary properties of the mixture in the very neighborhood of the phase envelope and the restrictive role of the spinodal surface as a boundary for possible equilibrium states with different pressures. (C) 2001 Elsevier Science B.V. All rights reserved.

**General information**
State: Published
Organisations: CERE – Center for Energy Ressources Engineering, Department of Chemical and Biochemical Engineering
Authors: Shapiro, A. (Intern), Stenby, E. H. (Intern)
Pages: 17-32
Publication date: 2001
Main Research Area: Technical/natural sciences

**Publication information**
Journal: Fluid Phase Equilibria
Volume: 178
Issue number: 1-2
ISSN (Print): 0378-3812
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
Effect of Low Permeable Porous Media on Behavior of Gas Condensate
Effect of low permeable porous media on behavior of gas condensates

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

Host publication information
Title of host publication: Proceedings of the European Petroleum Conference
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 176877
Publication: Research - peer-review › Article in proceedings – Annual report year: 2000

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

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering
Authors: Shapiro, A. (Intern), Stenby, E. H. (Intern)
Pages: 305-323
Publication date: 2000

Main Research Area: Technical/natural sciences

Publication information
Journal: Transport in Porous Media
Volume: 41
Issue number: 3
ISSN (Print): 0169-3913
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.16 SJR 0.767 SNIP 1.316
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.728 SNIP 1.317 CiteScore 1.94
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.932 SNIP 1.433 CiteScore 1.91
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.04 SNIP 1.433 CiteScore 2.03
ISI indexed (2013): ISI indexed yes
High Pressure Multicomponent Adsorption in Porous Media

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

Publication information
Journal: Fluid Phase Equilibria
Volume: 158-160
ISSN (Print): 0378-3812
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 2.33 SJR 0.869 SNIP 1.155
Nonequilibrium Segregation in Petroleum Reservoirs

General information
State: Published
Analysis of Multicomponent Adsorption Close to a Dew Point

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

Publication information
Journal: Journal of Colloid and Interface Science
Volume: 206
ISSN (Print): 0021-9797
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 4.14 SJR 1.144 SNIP 1.267
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.095 SNIP 1.263 CiteScore 3.8
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.166 SNIP 1.406 CiteScore 3.74
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.19 SNIP 1.45 CiteScore 3.73
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.298 SNIP 1.469 CiteScore 3.4
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.162 SNIP 1.419 CiteScore 3.3
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.279 SNIP 1.46
Web of Science (2010): Indexed yes
Potential Theory of Multicomponent Adsorption

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering
Authors: Shapiro, A. (Intern), Stenby, E. H. (Intern)
Pages: 146-157
Publication date: 1998
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Colloid and Interface Science
Volume: 201
ISSN (Print): 0021-9797
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 4.14 SJR 1.144 SNIP 1.267
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.095 SNIP 1.263 CiteScore 3.8
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.166 SNIP 1.406 CiteScore 3.74
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Kelvin Equation for a Non-Ideal Multicomponent Mixture

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

Publication information
Journal: Fluid Phase Equilibria
Volume: 134
ISSN (Print): 0378-3812
Ratings:
Effects of Capillary Forces and Adsorption on Reserves Distribution

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering
Authors: Shapiro, A. (Intern), Stenby, E. H. (Intern)
Pages: 1-8
Publication date: 1996
Conference: 1996 SPE European Petroleum Conference, Milan, Italy, 01/01/1996
Main Research Area: Technical/natural sciences

Publication information
Journal: SPE
Volume: 36922
Original language: English
Source: orbit
Source-ID: 168050
Publication: Research - peer-review › Journal article – Annual report year: 1996

On the nonequilibrium segregation state of a two-phase mixture in a porous column
The problem of segregation of a two-phase multicomponent mixture under the action of thermal gradient, gravity and capillary forces is studied with respect to component distribution in a thick oil-gas-condensate reservoir. Governing equations are derived on the basis of nonequilibrium thermodynamics. A steady state of the two-phase mixture with nonzero diffusion fluxes and exchange between phases is described. In the case of binary mixtures analytical formulae for saturation, component distribution and flow in the two-phase zone are obtained.

General information
State: Published
Organisations: CERE – Center for Energy Ressources Engineering, Department of Chemical and Biochemical Engineering
Authors: Shapiro, A. (Intern), Stenby, E. H. (Intern)
Pages: 83-106
Publication date: 1996
Main Research Area: Technical/natural sciences

Publication information
Journal: Transport in Porous Media
Volume: 23
Issue number: 1
ISSN (Print): 0169-3913
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.16 SJR 0.767 SNIP 1.316
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.728 SNIP 1.317 CiteScore 1.94
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.932 SNIP 1.433 CiteScore 1.91
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.04 SNIP 1.433 CiteScore 2.03
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Statistical Description of Segregation in a Powder Mixture

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

Principles of statistical physics are applied for the description of thermodynamic equilibrium in disperse systems. The cells of disperse systems are shown to possess a number of non-standard thermodynamic parameters. A random distribution of these parameters in the system is determined. On the basis of this distribution, it is established that the disperse system has an additional degree of freedom called the macro-entropy. A large set of bounded ideal disperse systems allows exact evaluation of thermodynamic characteristics. The theory developed is applied to the description of equilibrium states of a two-phase multicomponent mixture in a porous medium.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering
Authors: Shapiro, A. (Intern)
Publication information
Journal: Physica A: Statistical Mechanics and its Applications
Volume: 232
Issue number: 1-2
ISSN (Print): 0378-4371
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 0.782 SNIP 1.324 CiteScore 2.23
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.695 SNIP 1.131 CiteScore 1.94
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.657 SNIP 1.253 CiteScore 1.89
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.651 SNIP 1.168 CiteScore 1.79
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.667 SNIP 1.228 CiteScore 1.84
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.792 SNIP 1.066 CiteScore 1.7
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.881 SNIP 0.936
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.827 SNIP 1.037
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.817 SNIP 0.837
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 0.855 SNIP 0.992
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 0.804 SNIP 0.841
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 0.831 SNIP 0.818
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 0.811 SNIP 0.859
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 0.674 SNIP 0.714
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 0.714 SNIP 0.816
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 0.605 SNIP 0.801
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 0.929 SNIP 0.781
Scopus rating (1999): SJR 0.932 SNIP 0.721
Original language: English
DOIs: 10.1016/0378-4371(96)00137-9
Projects:

**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: Nielsen, Sidsel Marie (Intern)

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

**Gas liberation in tight porous medium**

Department of Chemical and Biochemical Engineering  
Period: 01/01/2018 → 31/12/2020  
Number of participants: 4  
Phd Student: Al-Masri, Wael Fadi (Intern)  
Supervisor: Nielsen, Carsten Møller (Intern)  
Nielsen, Sidsel Marie (Intern)  
Main Supervisor: Shapiro, Alexander (Intern)

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

**Advanced oil recovery processess: Modifications of injection water composition**

Department of Chemical and Biochemical Engineering  
Period: 15/02/2017 → 14/02/2020  
Number of participants: 3  
Phd Student: Hao, Jiasheng (Intern)  
Supervisor: Shapiro, Alexander (Intern)  
Main Supervisor: Nielsen, Sidsel Marie (Intern)

**Financing sources**  
Source: Internal funding (public)  
Name of research programme: Institut stipendie (DTU)  
Project: PhD
Enhanced Oil Recovery Methods targeting Danish North Sea Chalk Reservoirs

Department of Chemical and Biochemical Engineering
Period: 15/01/2017 → 14/01/2020
Number of participants: 3
Phd Student:
Taheriotaghsara, Mirhossein (Intern)
Supervisor:
Shapiro, Alexander (Intern)
Main Supervisor:
Nielsen, Sidsel Marie (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
Period: 01/09/2015 → 31/08/2018
Number of participants: 4
Phd Student:
Brand Ferrell, Justin (Intern)
Supervisor:
Stenby, Erling Halfdan (Intern)
Yan, Wei (Intern)
Main Supervisor:
Shapiro, Alexander (Intern)

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

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

Relations
Publications:
Phase Equilibrium Modeling for Shale Production Simulation
Project: PhD
Modelling of Salinity Effects on Waterflooding of Petroleum Reservoirs
Department of Chemical and Biochemical Engineering
Period: 01/09/2012 → 26/05/2016
Number of participants: 6
Phd Student:
Alexeev, Artem (Intern)
Supervisor:
Thomsen, Kaj (Intern)
Main Supervisor:
Shapiro, Alexander (Intern)
Examiner:
Nielsen, Sidsel Marie (Intern)
Berenblyum, Roman (Ekstern)
Mackay, Erik James (Ekstern)

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

Relations
Publications:
Modeling of Salinity Effects on Waterflooding of Petroleum Reservoirs
Project: PhD

Single Biomass Particle Combustion and Fuel Characterization
Department of Chemical and Biochemical Engineering
Period: 01/04/2012 → 18/08/2016
Number of participants: 8
Phd Student:
Trubetskaya, Anna (Intern)
Supervisor:
Jensen, Peter Arendt (Intern)
Jensen, Anker Degn (Intern)
Shapiro, Alexander (Intern)
Main Supervisor:
Glarborg, Peter (Intern)
Examiner:
Ahrenfeldt, Jesper (Intern)
Thunman, Henrik (Ekstern)
Wadenbäck, Johan (Ekstern)

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

Relations
Publications:
Fast pyrolysis of biomass at high temperatures
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

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

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD
Stochastic Modelling Polydisperse Transport of Particles in Porous Media

Department of Chemical and Biochemical Engineering

Period: 01/10/2009 → 17/12/2012

Number of participants: 6

Phd Student:
Yuan, Hao (Intern)

Supervisor:
Stenby, Erling Halfdan (Intern)

Main Supervisor:
Shapiro, Alexander (Intern)

Examiner:
Szabo, Peter (Ekstern)
Bradford, Scott Alan (Ekstern)
Lindeloff, Niels (Intern)

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

ParPor - Particles in Pores. Stochastic Modeling of Polydisperse Transport

Particle transport in porous media takes place in a range of contexts, i.e. industrial filtration, waste water treatment, mass transfer in human tissues, mud filtration around oil wells and others. Based on a stochastic approach the CERE project develops software for practical use in modeling of flows of suspensions in porous media.

Funded by FIST
DOC 09/01186

Center for Energy Resources Engineering

Department of Chemical and Biochemical Engineering

CERE – Center for Energy Ressources Engineering

Period: 01/09/2009 → 31/08/2012

Number of participants: 1

Acronym: ParPor
Project ID: 50711

Project Manager, academic:
Shapiro, Alexander (Intern)

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

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

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

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

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

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

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

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

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

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

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

Molecular Modelling of Polymer Melt Rheology
Department of Chemical and Biochemical Engineering
History Matcging using Stochastic Methods

Department of Chemical and Biochemical Engineering
Period: 01/09/2004 → 15/05/2008
Number of participants: 6
Phd Student:
Johansen, Kent (Ekstern)

Supervisor:
Stenby, Erling Halfdan (Intern)
Main Supervisor:
Shapiro, Alexander (Intern)
Examiner:
Michelsen, Michael Locht (Intern)
Hu, Lin Y. (Ekstern)
Mosegaard, Klaus (Intern)

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

Avanceret Reservoirsimulering

Department of Chemical and Biochemical Engineering
Period: 15/08/2004 → 16/05/2008
Number of participants: 7
Phd Student:
Kristensen, Morten Rode (Intern)

Supervisor:
Michelsen, Michael Locht (Intern)
Thomsen, Per Grove (Intern)
Main Supervisor:
Stenby, Erling Halfdan (Intern)
Examiner:
Shapiro, Alexander (Intern)
Aavatsmark, Ivar (Ekstern)
Saaf, Fredrik (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: DTU-lønnet stipendie
Project: PhD
**Phase Behaviour and Viscosity Modelling of Refrigerants-Lubricants Mixtures**

Department of Chemical and Biochemical Engineering  
Period: 01/11/2002 → 30/03/2006  
Number of participants: 6  
PhD Student:  
Monsalvo, Matias Alfonso (Intern)  
Supervisor:  
Thomsen, Kaj (Intern)  
Main Supervisor:  
Shapiro, Alexander (Intern)  
Examiner:  
Mollerup, Jørgen (Intern)  
Knudsen, Kim (Intern)  
Montel, Francois (Ekstern)  

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

**Transport Properties in Free Space and in aPorous Media**

Department of Chemical and Biochemical Engineering  
Period: 01/11/2001 → 04/03/2005  
Number of participants: 5  
PhD Student:  
Medvedyev, Oleg (Ekstern)  
Main Supervisor:  
Shapiro, Alexander (Intern)  
Examiner:  
Hassager, Ole (Intern)  
Lindeloff, Niels (Intern)  
Wesselingh, Johannes (Intern)  

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

**Compositional Streamline Simulation.**

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

**Financing sources**  
Source: Internal funding (public)
Transport Coefficients in Hydrocarbon Mixtures under Microgravity Conditions

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

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

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

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

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

Kompositionel reservoirsimulering af gas injektionsprocesser

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

Financing sources
**Modelling of Phase Equilibria and Transport Properties (C.1)**

Modelling of the phase behavior of reservoir fluids within a porous medium and during injection of gases.

Department of Chemical and Biochemical Engineering

Period: 01/01/1998 → 31/12/1998

Number of participants: 5

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

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

**Recovery processes (C.7)**

Experimental and theoretical investigations of oil recovery processes with emphasis on low permeable reservoir rocks.

Department of Chemical and Biochemical Engineering

Period: 01/01/1998 → 31/12/1998

Number of participants: 8

Project participant:
- Mogensen, Kristian (Intern)
- Poulsen, Søren (Intern)
- Dang, Tran Thuong (Intern)
- Poulsen, Susanne (Intern)
- Shapiro, Alexander (Intern)
- Ivar Andersen, Simon (Intern)
- Dandekar, Abhijit (Intern)

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