

Annual Report 2011





Technical University of Denmark



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an oil and gas reservoir.

Scientist.



**CERE Annual Report 2011** 

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## **Cover Photo:**

In 2011, CERE and partners were able to launch an ambitious program, BioRec, focused at enzymatic and microbial enhanced oil recovery. The picture shows interfacial tension (IFT) and contact angle experiments under the program. Experimental setup: Alsu Khusainova, CERE DTU Photo: Christian Carlsson, CERE DTU

## A New Flavour to Oil Recovery

In its second year, CERE was able to launch new large projects and

BioRec (Biotechnology in Oil Recovery) is a large new research program aiming to provide the foundation for microbial and enzymatic enhanced oil recovery.

Modifications like changing salinity may increase yields from water flooding in oil recovery significantly. An ambitious new program aims to optimize the method.

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Erling H. Stenby Chairman of CERE, professor ehst@kemi.dtu.dk

# **Our Transition** is completed

The integration of scientific capabilities from a number of DTU departments into CERE can already be claimed a success.

ust two years ago we embarked on a journey, as academic staff from a number of DTU departments were welcomed in the Center for Energy Resources Engineering. Without weakening our traditional strongholds from IVC-SEP, we have been able to smoothly integrate faculty members and other scientific staff from DTU Chemical Engineering, DTU Informatics, DTU Civil Engineering and DTU Chemistry.

The prime ambition behind the expansion was to position ourselves strongly in the competition for funding of large, highly interdisciplinary research programs. I am pleased to say that our industry stakeholders and the bodies responsible for public research funding have responded positively.

Already in our second year as CERE, 2011, we were able to initiate several novel research projects. As these will be thoroughly presented over the following pages, I will not go into details here but limit myself to underlining one common feature. The new projects are interdisciplinary, and not least do our new resources within geology and geophysics contribute strongly.

## Shale gas and HPHT

Looking ahead, I am convinced that the enhanced possibilities inherent in our new structure have in no way been exhausted. Let me just point to a few possible future areas for us. The current US administration has a strong focus on shale gas, which again has spurred wide research activity. The potential for shale gas reservoirs in Denmark is highly interesting, and CERE is well positioned in possible efforts to exploit them.

Similarly, HPHT (High Pressure, High Temperature) oil and gas reservoirs are currently at high focus in the Mexican Gulf, but they are found in the Danish part of the North Sea as well. In both contexts, an interdisciplinary approach found at page 30.

involving applied chemistry, chemical engineering, geology and geophysics will be essential.

The same is true for heat storage in deep aquifers, possibly combined with geothermal energy exploitation. A large Danish research project coordinated by CERE is in progress (see our Annual Report 2010) and activity is expected to increase over the coming years.

## Guarding our core activities

In closing I would like to stress that, even as excited as we are about the range of new fields and projects opening to us, we have not forgotten where we came from. The core activities of CERE have been, and will always be, central scientific disciplines such as applied thermodynamics, scientific computing, rock physics and applied chemistry.

Whenever we cooperate with academic staff across DTU you will always be able to find a link between their work and CERE core disciplines, thus adding to the synergy between various DTU departments and obtaining increased value from the resources at hand. In this respect by "resources", I am thinking both of academic staff and of the time we are grateful to be able to spend at advanced research equipment at the various DTU departments involved.

Summing up, we are well positioned for the challenges ahead and look forward to engage in even closer cooperation with our stakeholders in the years to come.

> Professor Erling H. Stenby, Chairman of CERE

A more detailed summary of 2011 events to be

# The Consortium our Strongest Asset

**C**ERE is supported by public means from several sources, e.g. The Danish Research Council for Technology and Production Sciences and The Nordic Energy Research Programme. Furthermore the Center is supported by grants from several private companies. The strongest asset of CERE is the industrial Consortium. Approximately 25-30 companies are members, the exact number changes due to the

dynamics of the industry's mergers and acquisitions. The member companies closely follow the activities of the Centre. This ensures that CERE activities are relevant in relation to the topical problems and limitations in existing knowledge within applied thermodynamics. This ongoing external control of quality and inspiration assist in maintaining CERE research at the highest international level.



## **CERE** Consortium:

- Statoil Maersk Oil Gaz de France ConocoPhillips Haldor Topsøe BP SOM Linde Total ●
- Eni 

  DONG Energy

  Shell

  GASSCO

  OMV

  Chevron

  Petrobras

  RWE

  Akzo

  Nobel

  IFP

  Schlumberger

CERE's Discussion Meeting is a unique opportunity for Consortium participants and researchers from the Centre to interact. The *2011 version (picture)* set a new record in industry participation.

• ExxonMobil • Vattenfall • Welltec • Saudi Aramco • Sinopec • Lloyd's Register ODS • NKT Flexibles •

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# Novel Green Tools in Oil Recovery

It is known that certain microbes are able to increase recovery rates. The question is whether Microbial Enhanced Oil Recovery (MEOR) and possibly enzymatic enhanced oil recovery can be utilized in a practical and economically feasible way. A large new Danish research programme addresses North Sea reservoir applications, while aiming to increase the general understanding of the subject.

n a joint effort with two Danish energy corporations, Maersk Oil and DONG Energy, and the world's leading enzyme producer, Novozymes, CERE embarks on an ambitious quest. The BioRec program aims to create the scientific foundation for introducing microbial and enzymatic enhanced oil recovery (EEOR) methods in full-scale recovery.

"Everywhere around the world oil reserves

are diminishing. This again drives up oil prices, giving industry more incentive to apply less trivial recovery methods. While MEOR and EEOR are still in a scientific state, with very few field tests, it is likely that the methods we are looking at will be applied as the present trend in oil prices continue," says the coordinator of the MEOR work package in BioRec, Associate Professor Alexander Shapiro, CERE.

## Microbes to the rescue

As the rest of the BioRec project, the MEOR component is focused at oil fields in the Danish part of the North Sea.

"Production in the Danish part of the North Sea is diminishing, but not so much because the reserves have been expired but rather because we simply do not know how to extract the majority of the oil. Present methods may yield a final recovery rate of about 25 per cent. Just a few per cent increase in that rate would more than justify the cost of the research programme," Alexander Shapiro says, while adding:

"And of course we hope to find methods that will increase production more than just marginally."

The geological conditions in the Danish part of the North Sea - dominated by dense chalk reservoirs - are the main reason why expectations for the overall recovery rate have to be modest at present. For instance, roughly half of known oil reserves in the Danish part of the North Sea are found in chalk with extremely low permeability from the so called Danian periode.

Enhanced Oil Recovery (EOR) is a way to extend the productive life of an otherwise depleted and uneconomic oil field. EOR is usually applied after more conventional methods, primarily pressure depletion and water flooding, have been exhausted. While most commonly either water or gas is injected into the reservoir - over the latest years MEOR has gained increased attention.

## Bacteria in oil are strange creatures

Manipulating microbiology is actually not unknown to the oil industry. For example in some fields, where growth of naturally occurring sulphur-reducing microbes would cause problems, it is an established method to inject nitrate-rich sea water. This stimulates growth of nitrate-reducing microbes which again limits the potential growth of sulphur-reducing microbes. Still, the idea of actively using microbes to increase production is less than 3 years old.

At the initial stage, the BioRec program aims "to solve an old puzzle", Alexander Shapiro reveals:

"We know that bacteria live in oil reservoirs in the North Sea. They are pretty strange creatures, able to survive and be active without oxygen, BioRec

Stenby.

The programme has an overall budget of EUR 4.5 million, where EUR 2.0 million has been provided by the Danish Advanced Technology Foundation, EUR 1.5 million by the industry partners and the last EUR 1.0 million by DTU.

under temperatures of around 80° and pressures above 100 bars. However, it is not clear how it is possible, since the pores are roughly the same size as the bacteria, and the bacteria often exist in colonies. So: how deeply do they penetrate the porous rock? How do they form colonies? These questions are to be addressed in a series of advanced experiments on bacterial flooding of reservoir core samples."

"With regard to enzymes, the first step in the project is to check whether they can change the preference of the rock surface to oil or to water. In the reservoirs oil may "stick" to the surface - that is why it is so difficult to extract. The mixtures of enzymes and surfactants may separate oil from the surface, make it more water-wet. This is what enzymes do, for example, in washing powder."

## Which bacteria to bet on?

In MEOR, either bacteria are injected together with nutrients or indigenous bacteria are activated by injection of nutrients.

"The latter method is of course tempting as we know that bacteria already live in the reservoirs and thus are able to sustain the conditions. Even under extreme reservoir conditions bacteria can produce biopolymers and biosurfactants, change acidity of the reservoir water, plug waterflooded zones of a reservoir and do other important jobs for enhancing the recovery. We know that at least 10 species exist in quantities above 1-2 per cent of the total population. We need to have a better understanding of the mechanisms involved in order to determine which of these is "the horse we should

The BioRec program (Biotechnology in Oil Recovery) consists of three work packages. The package on microbial and enzymatic oil recovery is coordinated by Associate Professor Alexander Shapiro, CERE, while the package on inhibition of gas hydrate formation by antifreeze proteins is coordinated by Associate Professor Nicolas von Solms, CERE, and the package on prevention of microbial induced corrosion by DTI. Overall BioRec coordinator is CERE Chairman, Erling H.

*The image shows* crude oil droplets attached to a solid surface. A core activity in the BioRec program is to investigate how en*zymes and surfactants* produced by microbes will alter the shape of oil droplets and their attachment to the surrounding rock.

We were able to use some of our existing equipment and are also purchasing several new instruments. As a result we are able to do things that not many other labs in the world could do." **Associate Professor** Alexander Shapiro, CERE

bet on"," says Alexander Shapiro, continuing:

"MEOR methods are not widely used commercially. It is known that several species of bacteria are able to increase recovery rates, but so far experience has mostly been from practical trials. You inject bacteria into a reservoir and wait a few days or months to see if production will increase or not. If it increases, well, that's good news but we would also want to know why. What is the mechanism? Without this understanding we can hardly hope to be able to optimize the method and to understand when and where it can be successfully applied."

## Surfactants reduce interfacial tension

A range of possible mechanisms can be imagined to be related to the efficiency of MEOR. One is reduction of the interfacial tension (IFT) due to surfactant production. In a recent study, Post Doc Sidsel Marie Nielsen, CERE, has demonstrated that surfactants produced by microbes are capable of increasing incremental recovery significantly compared to water flooding.

As a part of the BioRec programme she and her colleagues at CERE will continue these studies. A number of rock types known from the Danish part of the North Sea have be saturated with oil. Lab trials are hoped to show both how much recovery can be increased and how much of this increase can be attributed to bacteria's production of surfactants.

Another mechanism of interest is linked to so called biofilms. Under the right conditions bacteria will form biofilms consisting of a mixture of the bacteria themselves, particles and substances produced by the bacteria serving as



nism behind the efficiency of microbial enhanced oil recovery (MEOR) is reduction of the interfacial tension (IFT) due to sur*factant production by* the microbes. A range of interfacial tension studies will be carried out.

a kind of glue. Biofilm formation may increase the MEOR recovery rate further - this is believed to be related to microscopic fluid diversion as a part of the overall fluid diversion mechanism due to the formation of biofilm.

Also several other mechanisms might play a role in increasing oil recovery. In Sidsel Marie Nielsen's recent simulation studies a total improvement in the recovery rate against water flooding of 15 per cent of the oil that was originally present, was achieved at optimal conditions by a combination of several mechanisms. Sidsel now holds a dual role as both post doc and the overall project manager of the BioRec project.

## Purchase of non-standard equipment

In the ongoing studies it seems possible to increase recovery rates further by adding enzymes to the solution. While these results are promising, there

## Novozymes: The potential could be promising

To some it may seem as a surprise to see the world's leading producer of enzymes involved in a program related to oil and gas recovery.

"It is always interesting for Novozymes to have enzymes tested within a new industrial framework," explains Science Manager Hanne Høst Pedersen of Novozymes R & D, adding:

"The very first step would be to achieve proof of concept, meaning to show that an enzyme or a microbe could actually play a role in increasing oil recovery. The next step would be to start optimizing this type of enzyme to really fit the application. We have thousands of enzymes and microbes in our collections of which only a small fraction have ever been transformed into commercial products - so we have plenty to pick from.

BioRec gives us the possibility to have biotechnology based solutions tested in laboratory models at relevant downhole working conditions i.e. setups we would never be able to run in Novozymes' own laboratories, and we also get the important close contact to the potential final end user companies operating in the field."

Use of enzymes in oil recovery is still at an early stage, underlines Helle Simon Elbro, Business Development Manager, Novozymes

"We are scouting for possible business opportunities by screening rather broadly among different types of enzymes. The road to something that could become a commercial product is very long. On the other hand, should business opportunities arise at some point, the potential could be promising."

is still quite a distance to go before the method can be practically used, Alexander Shapiro stresses:

"It appears to be possible to achieve significant increases in recovery by injecting solutions containing about 5 per cent of enzymes and 10-15 per cent of surfactants. Obviously this in encouraging but we have to realize that 5 per cent of enzymes is not that little. As your average oil reservoir would be about the size of a city, you would need a large quantity of enzymes to cover the entire reservoir. This would be too expensive. So we need to do something. One approach could be to find a smarter way of injecting so we don't need to cover the entire area. Another approach could be a form of recycling the enzymes. Finally, we might hope that lower concentrations would be able to do the job."

The financial contributions from the Danish Advanced Technology Foundation and the parties involved have made it possible to acquire several pieces of new laboratory equipment.

"Equipment for investigating effects of water flooding in oil fields is pretty standard and the same goes for methods for investigating the fate of bacteria in various media, but the combination of these two techniques is non-standard. There are specific questions that should be addressed: how to create anaerobic conditions, how to maintain hot temperature in the flooded samples, but instantaneously cool down the produced liquids in order to suppress post-experimental bacterial activity, how to measure distribution of bacteria in the rock samples, and many other. We were able to use some of our existing equipment but are also purchasing several new instruments. As a result we are able to do things that not many other labs in the world could do," Alexander Shapiro states.

## Mechanisms of universal relevance

While the prime focus is the North Sea it may be possible to apply some results to fields elsewhere, the BioRec WP1 coordinator hopes:

"On the one hand the conditions in the North Sea fields are complex both regarding mineralogy and the microbiological environment and characterized by non-trivial mechanisms, so there is no guarantee that a method working here could be directly transferred to other parts of the world. One the other hand our research is oriented towards mechanisms, so there is a good chance that the experience and the insight we gain will also have a more universal relevance."

Alexander Shapiro also chairs DTU's educational activities within petroleum engineering, for which BioRec is also an inspiration:

"Training already includes lectures on

sustainability but I am wondering whether our education should be diversified further. It seems to me that some biological aspects and bio-enhancement in oil recovery specifically have relevance to future petroleum engineers."

biology.

## Danish, but internationalized

The programme includes 3 CERE faculty members (the centre's Director Erling Stenby, Associate Professor Alexander Shapiro and Associate Professor Nicolas von Solms), 3 Post Docs (Sidsel Marie Nielsen, Sara Sandersen and Igor Nesterov) and 3 PhD-students (Alsu Khusainova, Christine Malmos and Amalia Halim). Besides obviously Danish staff, the programme has associates from Russia (trained in the UK), Indonesia (trained in Australia) and has a standing cooperation with a Russian petroleum engineering group working on microbiology of Chinese petroleum reservoirs.



This diversity is reflected in the BioRec scientific staff that covers chemistry, chemical engineering, applied mathematics and micro-

"So even though BioRec is focused at the Danish part of the North Sea, we have chosen to also gain from internationalizing the programme. As MEOR is an emerging field we find it important to keep an open mind to ideas and methods being developed in different countries and under different academic traditions," says Alexander Shapiro, while emphasizing that the project also draws on industry's research capacity.

BioRec gives us the possibility to have biotechnology based solutions tested in laboratory models at relevant downhole working conditions, i.e. setups we would never be able to run in Novozymes' own laboratories, and we also get the important close contact to the potential final end user companies operating in the field. **Science Manager** Hanne Høst Pedersen, Novozymes R & D

Equipment for investigating effects of water flooding in oil fields is standard and the same goes for methods for investigating the fate of bacteria in various media, but in combining these two techniques CERE needs to develop new methodologies.



# PhD Defense Upscaling of the Two-Phase Flows in Petroleum Reservoirs



Xuan Zhang, PhD Supervisor: Alexander Shapiro



Cimultaneous two-phase immiscible flows in water flooding – or displacement of oil by water **J**porous media arise in a number of processes in nature and industry. So called displacement flows are of great interest in engineering. Most of the research activity in this field is driven by the needs of the petroleum industry, and its desire to understand the dynamics of multiphase flow.

Multiphase flow modelling is extremely complex. Since it is not possible to obtain very detailed information about heterogeneous reservoirs, and computations accounting for all details of the reservoir structure are prohibitively timeconsuming, up-scaling techniques are needed to get pseudo-properties of the reservoirs: pseudo relative permeabilities and pseudo fractional flow functions. These functions define average effective properties on a large scale, based on small-scale properties and their distributions.

This project presents a semi-analytical upscaling method. Many petroleum reservoirs may be approximated by layered models where the variation of reservoir properties orthogonal to the reservoirs' areal extent is larger than that in the direction of the areal extent.

One of the oldest and most widely studied industrial processes in petroleum engineering is



in petroleum reservoirs. This is the most widely used and fundamental process for secondary oil recovery. Other methods for enhanced oil recovery (EOR), for example chemical flooding (surfactant, polymer), thermal flooding (steam, hot water) and gas flooding (air, carbon dioxide), are based on similar physical processes.

The efficiency of an oil recovery method is to a large extent determined by physical mechanisms at the microscopic level, e.g. how the phases - oil, water and gas - distribute in the pore space of the geological rock. Prediction of macroscopic (field scale) properties of a petroleum reservoir – such as water cut, oil recovery curve, inter-layer communication - directly determines the selection of recovery methods.

In the project a fast semi-analytical 1D simulation method for two-phase immiscible incompressible flow in a layer-cake reservoir has been developed. It may be used for up-scaling of water flooding in a stratified reservoir of a viscous dominant regime. The essence of the proposed method is to reduce the problem of 2D two-phase immiscible incompressible flow to the multiple 1D flow equations under the assumption of perfect inter-layer communication or, equivalently, vertical equilibrium.

For cases where the gravity effect is negligible, the results obtained by the method are very close to results obtained from complete 2D displacement simulation, in both well defined multilayer reservoir models, as well as the models with log-normal distributed permeabilities. For the cases where gravity is not negligible, the error of the method increases, but recovery is still calculated with reasonable accuracy.

Comparison with 2D Simulations: Water saturation profile for 2D waterflooding simulation, at time=0.25 p.v.i. The horizontal axis is the dimensionless distance along the reservoir, and the vertical axis is the dimensionless height (across the reservoir). M = 0.33.



# Smart Water Flooding - it Works, but why?

Injection of water has been used in oil and gas recovery for decades. However, recent findings suggest that changing salinity or making other modifications to the injected water may increase yields significantly. An ambitious new program aims at understanding the mechanisms involved in order to optimize the method.

hile water flooding is an absolute standard method used by oil companies all over the world every day in order to extract extra oil from mature fields, the theoretical understanding of the detailed mechanisms involved has never been developed to the same level. A new program - SmartWater - aims to change the scene.

"By the end of the program's four year period we will present a recipe, which companies can use for pilot trials," promises program coordinator Professor Ida L. Fabricius, CERE.

"If the program results in just a small increase in the yields from recovery, the economic effect to the companies involved and to the Danish society could be large."

A bit unusually, the program was proposed by the industry partners - Danish energy corporations Maersk Oil and DONG Energy. CERE was keen to accept the challenge.

"While a few other institutions may have published more on water flooding than we have, a fully satisfying explanation to the mechanisms involved has not been presented. We believe that we possess the right blend of expertise from chemistry, geology, chemical engineering and mathematics for the task. In my opinion it will be very important to keep an open mind as to

program.

Maersk Oil - MOG 1 Photo: Maersk

SmartWater has a budget of approximately 2.5 million EUR. Half is provided by the industry partners, while the other half stems from the Danish EUDP program (a program for development and demonstration of energy technology) under the Danish Energy Agency and the Danish research councils. CERE contributes with academic staff. The present budget allows for SmartWater to run until 2015. CERE Chairman, Erling H. Stenby, is overall responsible for the

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which scientific field - or fields - may hold the key to the explanation we are looking for," says Ida L. Fabricius.

## Sweet water works in sand

The program is focused on the Danish part of the North Sea. However, the inspiration was found in a different part of the world, in the Middle East, where injection of sweet water instead of the usual salt water proved to increase yields in sand reservoirs.

"It seems that using water with a salinity which differs from the salinity of the water present in the geological structures containing a reservoir does have a desirable effect. However, we would of course very much like to know why in order is nuclear magnetic resonance (NMR) spectroto propose the optimal way to modify the water for a given field," Ida L. Fabricius explains, while adding that just using sweet water is not likely to be the best solution in the Danish part of the North Sea.

Sea are very different from sand reservoirs in the Middle East, different solutions could be needed."

Also, salinity is not the only focus of Smart-Water, she stresses:

"Once we understand the mechanism, we may be able to suggest other modifications like having specific ions in your water. Obviously, these would have to be available in a cost-effective manner, but still we have some options."

## Chalk and greensand

SmartWater is focused at two types of sedimentary rocks in the Danish part of the North Sea, chalk and greensand.

North Sea chalks are composed of micrometer sized fossils which are developed from the diagenesis of pelagic calcareous ooze. Due to small particle size, the chalk has a homogeneous structure with high specific surface area. The high specific surface of particles means that the solid has large exposure to the fluid – be it either oil or first can be very complex." water from water flooding.



Greensands are composed of a mixture of stiff Besides chalk, the clastic quartz grains and soft glauconite grains. Glauconites are porous and composed of aggregates of iron-bearing clay. Greensand petroleum greensands (pictureservoirs can be found all over the world.

Samples of both types of rocks will be analyzed *composed of a mix*in new advanced flooding equipment at CERE. Samples will be provided by Maersk Oil and DONG Energy, while sample saturation will be provided by the Geological Survey of Denmark and Greenland (GEUS).

## An element of academic competition

One type of investigations which the project coordinator holds exceptionally high hopes for scopy.

"The NMR scans will allow us to map both the pore size inside a sample and the distribution of oil and water. In addition we hope to be able to establish whether oil or water is in contact with "As the geological conditions in the North the wall of the pores," says Ida L. Fabricius.

> Besides herself, Associate Professor Alexander Shapiro, Associate Professor Kaj Thomsen and Assistant Professor Philip Fosbøl are the faculty presently involved in SmartWater. Monzurul Alam participates as a Post Doc. Hiring for an additional position as Post Doc and three PhD positions is in progress.

The four present faculty members have very different backgrounds, and Ida L. Fabricius - a geologist herself - does not hide an element of can use for pilot competition in the group to come up with the trials. If the program best explanation to the mechanisms involved in water flooding:

"Some of us have our pet theories. I am not going to tell you what my own theory is, because I really wish to keep an open mind at this early stage. It is intriguing that at the one hand we have promised to provide a very simple product, which is a recipe for pilot projects in the North Sea, but on the other hand the theory we need to develop

SmartWater program will focus on re). Greensands are ture of stiff clastic quartz grains and soft glauconite grains. Glauconites are porous and composed of aggregates of ironbearing clay.

By the end of the program's four year period we will present a recipe, which companies results in just a small increase in the vields from recovery, the economic effect to the companies involved and to the Danish society could be large. Professor Ida L. Fabricius, CERE

# PhD Defense Rock-physics modelling of North Sea greensand

reensands are composed of a mixture of rock-physics modelling in the project indicates that stiff clastic quartz grains and soft glauconite grains. Glauconites are porous and composed of aggregates of iron-bearing clay. While greensand petroleum reservoirs can be found all over the world, evaluation of these reservoirs remains a challenge to geologists, engineers and petrophysicists.

In the project, greensands from the Hermod Formation and the Ty Formation in the Nini field of the North Sea were studied by a series of laboratory experiments including core analysis, capillary pressure measurements, NMR (nuclear magnetic resonance), acoustic velocity measurements and electrical properties measurements. Also CO<sub>2</sub> injection experiments were done, just as thin sections and BSE (backscattered electron micrographs) images were available.

Zakir Hossain, PhD

Initially greensand is

a mixture of mainly

quartz and glauconi-

takes place greensand

properties will chan-

ge. Various rock-phy-

sical models were de-

veloped in the project

to predict changes in

elastic properties and

other factors.

te. As cementation

Supervisor:

Ida L. Fabricius

The central part of the study is rock-physics modelling of greensand. Rock-physics modelling is becoming an integral part of geophysics, petrophysics and geology. Rock-physics modelling bridges the elastic properties and the geological properties.

Combined with thin section observations, the fine pore-filling materials.





variations in the elastic properties of greensand can be explained by two main diagenetic phases: silica cementation and berthierine cementation.

Initially greensand is a mixture of mainly quartz and glauconite. As cementation takes place greensand properties will change. Various rock-physical models were developed to predict changes in elastic properties and other factors. NMR studies were used to describe the fluid related dispersion in greensand.

In the final part of the study CO<sub>2</sub> injection effects on physical properties of greensand were investigated. Laboratory results indicate that CO2 injection has no major effect on porosity, electrical properties and elastic properties of greensand. In contrast, permeability increased after CO<sub>2</sub> injection. An NMR permeability modelling approach was used to evaluate the effect on matrix permeability of CO<sub>2</sub> injection. It appears that permeability after CO<sub>2</sub> injection increased not due to fracturing but rather due to an increase of macro-pores in the greensand. The increase of macro-pores size is probably due to migration of

# CO<sub>2</sub> Injection in Chalk

Mohammad Monzurul Alam, PhD. Today works at CERE as Post doc Supervisor: Ida L. Fabricius

rhanced oil recovery (EOR) by injecting **C**supercritical CO<sub>2</sub> in depleted hydrocarbon reservoirs addresses two global issues at the same time: reducing CO<sub>2</sub> in the atmosphere and increasing oil production. Chalk reservoirs in the Danish part of the North Sea are of particular interest for applying this method. Because of high porosity the storage capacity of these chalk reservoirs are high, while on the other hand conventional oil recovery processes like water flooding are less effective.

**Rock Physical Aspects of** 

PhD Defense

As CO<sub>2</sub>-EOR is a relatively new method a range of questions need to be answered regarding the impact of injection to the physical composition of the chalk. Among other methods, the project used sonic velocity measurements to study permeability and other key features.

In the project, the impact of supercritical CO<sub>2</sub> on the petrophysical and rock-mechanics properties was investigated on samples from the Ekofisk Formation and the Tor Formation chalk from South Arne Field, Danish North Sea. The chalk is characterized by high porosity and

low permeability. Injection of supercritical CO<sub>2</sub> increases mobility of the oil and at the same time high porosity provides large storage capacity. A series of laboratory experiments were focused at changes in porosity, specific surface, pore stiffness, wettability, mineralogy and mechanical failure.

In order to understand the development of chalk from calcareous ooze and achieving pore stiffness, the diagenesis process of a sedimentary sequence from Kerguelen Plateau in the Indian Ocean was studied.

Reservoir compaction is a result of both elastic and plastic deformation, while sound velocity only characterizes elastic properties of rocks.

Due to supercritical CO2 injection a 2-3 per cent increase in porosity was observed, just as a minor smoothening of particle surfaces and a consequent small increase in permeability and a decrease in elastic stiffness. No significant increase in wettability was noticed. It was found that the effect of CO2 injection on both petrophysical and mechanical properties of chalk depend on carbonate content. Pure chalk with high carbonate content is relatively prone to mechanical weakening due to CO2 injection, while no significant effect was observed in relatively impure chalk from the Ekofisk Formation. In spite of mechanical weakening only minor compaction is expected because effective stress is decreased due to an increase in effective stress coefficient.

Extensive time-lapse monitoring strategies are required during a CO<sub>2</sub>-EOR process for the measurement of changes in reservoir properties that may cause deformation of and leakage from a reservoir. The results of this study will provide data for designing future monitoring strategies based of 4D seismic measurements.

Injection of supercritical CO<sub>2</sub> increases mobili*ty of the oil and at the same time high porosity* provides large storage capacity. A series of laboratory experiments were focused at changes in porosity, specific surface, pore stiffness, wettability, mineralogy and mechanical failure.



# A Dedication to Carbon Capture

By hiring Philip Fosbøl to a new faculty position as Assistant Professor, CERE marks a further upgrade of its CCS (Carbon Capture and Storage) activities.

Much like the tide varies between high and low, so does the political focus on carbon capture go up and down. Still, CERE's commitment to the field remains unchanged. The latest confirmation of this fact is the hiring of Philip Fosbøl for a new Faculty position as Assistant Professor.

With a background of writing his Masters at CERE, then working firstly as a PhD student and later as a Post Doc, Philip Fosbøl was already an established figure at the centre as he entered the new position by December 1st 2011. Still, by choosing him for the position CERE reaffirms its commitment to CCS research. While topics and angles in his previous projects have differed, carbon dioxide has been the common denominator for most of them.

"Obviously the outlook for CCS is closely linked to the discussions over the future of coal. Some countries are aiming directly for a green









energy future and may thus not presently see a need for a cleaner form of coal based energy. However, on a global scale it is evident that coal will play a large role for many years and also, that carbon capture will be implemented," says Philip Fosbøl.

## Europe looking to "decarbonise"

To justify an ongoing CCS focus one needs only to look at the energy policies of the EU. The union has committed to a 20 per cent reduction of carbon emissions by 2020, and sees CCS as a necessary means.

"Reinventing our carbon intensive infrastructures is critical if we are to meet our EU and global climate change objectives. Achieving emissions cuts of 80-95 per cent below 1990 levels by 2050 requires a process of "decarbonising" the economy. For this to materialise new and innovative low-carbon technologies will have to be developed and deployed," according to the web page of the Directorate-General for Climate Action (DG CLIMA), going on to state:

"DG CLIMA makes sure that innovative technologies are deployed safely and that their risks are properly managed. The main issue here concerns carbon capture and storage (CCS) which



along with energy efficiency and renewable energy technologies, is expected to make an important contribution to meet global greenhouse gas emission targets."

The EU efforts are coordinated by the so called CCS Project Network. The aim is to have a number of demonstration projects running by 2015 and commercially viable CCS by 2020.

## Increasingly international in scope

CERE takes part in a number of CCS projects funded by EU sources, among them the Framework 7 program "iCap" - where the "i" is for "Innovation". While Norwegian university NT-NU is the overall coordinator, CERE coordinates the core of five work packages. The work package involves thermodynamic modelling. In other words the participating CERE researchers are the link between experimental results and later simulations done by other partners in the program.

The next EU initiative coming up is to be DG CLIMA's demonstration support initiative, the NER300 funding programme. The programme is expected to provide substantial funding for large-scale demonstration of low-carbon energy technologies in Europe and will be the world's largest programme in this area.

"Naturally we are keen to participate. Through iCap and other EU programmes and projects we already have collaboration with a large number of companies and academic partners in Europe. We expect our CCS activities to become increasingly international in scope," Philip Fosbøl comments.

## Chilled ammonia - hyped for a reason

Unlike many other scientists working with carbon capture, Philip Fosbøl hasn't yet picked a favourite capture technology. His works up till now have included practically all known solvent based capture techniques and even a few that are still only sketches. Thus he is able to give a fairly objective overview of the status of the various techniques which might challenge the well established method of capturing carbon dioxide using alkanolamines as solvent.

Firstly he points to the "chilled ammonia" process. Chemically speaking ammonia is a suitable solvent for carbon capture, but at room temperature ammonia would vaporize from the solution. Therefore ammonia has to be added in chilled and pressurised form.

"The chilled ammonia has been "hyped" quite a bit lately, but actually this has some justification. A major advantage is the fact that ammonia is a light molecule, meaning that you have a high capacity for transporting carbon dioxide per weight



unit of solvent. This again means less energy consumption for pumping. Another advantage is that the solvent is inexpensive, and it does not decompose on reaction. The downside is that the cooling represents some practical challenges and extra costs as it requires energy. Still, the chilled ammonia process is considered well advanced and it could be one of the competing technologies to challenge alkanolamine processes in the near future," the newly appointed Assistant Professor states.

## Ionic liquids and amino acids

Another CERE project - carried out in cooperation with DTU Chemistry - addresses ionic fluids. Professor Rasmus Fehrmann and colleagues at DTU Chemistry have previously been successful in utilizing ionic liquids for sulphur dioxide capture. This fostered the idea of using ionic liquids for capturing carbon dioxide in cooperation with CERE's experts.

Initial studies are promising, according to Philip Fosbøl:

"Unlike practically all other solvents the ionic liquids have the significant advantage that they are unable to vaporize. Even if heated they remain and are ready to be used again and again. The downside is that they are relatively heavy so you need to apply more energy for pumping. But then again, it is a quite new field and I still see many opportunities for further development." Also a number of other techniques - some still at an early stage of development – may enter

the scene.

"All have their own qualities. Take for instances the novel technique of using amino acids as solvent. Most amino acids are completely safe in relation to human health - some are even nutritional! Thus their advantage in respect to both the external environment and work environment is evident."

## Corrosion needs to be addressed

Besides the various innovative techniques CERE also maintains a focus on optimization of the present number one technique, which is alkanolamines.

"It is harder than ever to predict which this subject now." technique will be proven to be the best," Philip Fosbøl sums up.

For industry and academia faced with decisions regarding capture techniques the team at CERE has developed a software tool, the "CapCO<sub>2</sub>". The software is already available to CERE industry Consortium members.

Philip Fosbøl is the main contributor to "CapCO<sub>2</sub>" but stresses that he doesn't want to

## EU Carbon Capture Initiatives

Under the European Economic Recovery Programme around one billion EUR are allocated to CCS (Carbon Capture and Storage) demonstration.

The Directorate-General for Climate Action (DG CLIMA) is the EU's primary responsible entity for CCS activities.

DG CLIMA's upcoming demonstration support initiative, the NER300 funding programme, is expected to provide substantial funding for large-scale demonstration of low-carbon energy technologies in Europe and will be the world's largest programme in this area.

The Directorate-General's web site describes the role of CCS as: "Carbon capture and geological storage is a technique for trapping carbon dioxide as it is emitted from large point sources, compressing it, and transporting it to a suitable storage site where it is injected into the ground. The technology of carbon capture and storage has significant potential as a mitigation technique for climate change, both within Europe and internationally, particularly in those countries with large reserves of fossil fuels and a fast-increasing energy demand."

spend all his time in software development:

"I have always split my time between the lab and the computer. Both are important in what we do."

While keeping an open mind regarding capture techniques he admits to have a current pet focus of a different kind:

"I hope to be able to initiate research in corrosion prevention. It is well known that carbon dioxide is highly corrosive. No matter which technique will be chosen for capture we will always face a challenge of transporting carbon dioxide and thus also a risk of corrosion in pipes and other equipment. We might as well address



Victor Darde, PhD

Today works with

DONG Energy

Supervisor:

Kaj Thomsen

Aqueous Ammonia hilled ammonia has gained attention as a possible alternative to alkanolamine based techniques for post combustion carbon capture at power plants. The project investigates the

performance of two chilled ammonia capture

CO<sub>2</sub> Capture using

PhD Defense

solutions. Chemical absorption of carbon dioxide using amines is a well established process with years of experience around it, and it can be retrofitted to existing power plants. Thus, alkanolamine-based post-combustion capture (PCC) is considered state of the art technology for CO<sub>2</sub> removal from flue gases. The most commonly used amine is MEA, monoethanolamine.

However, use of amine solutions is associated with high heat consumption (3,500-4,000 kJ/kg  $CO_2$ ) and a high degradation rate of the amines - both factors contribute to higher costs. Thus it would be highly interesting to consider alternative capture techniques.

Capture using aqueous ammonia exists in two variant. The first variant absorbs the CO<sub>2</sub> at low



Using the Extended UNIQUAC model for the CO<sub>2</sub>-NH<sub>3</sub>-H<sub>2</sub>O system proposed by Thomsen and Rasmussen (1999) the project undertook thermodynamic studies of both CAP techniques. According to these studies, the heat requirement in the desorber was 1,850 kJ/kg  $CO_2$ . This is significantly lower than for the MEA process. However, the study also showed a high vapour pressure of ammonia in the absorber and thereby a need for extensive washing sections.

stripper, and the lowest total heat requirement for the desorber and the NH<sub>3</sub>-stripper found in the study was 2,700 kJ/kg CO2. So still well below the heat requirement for the MEA process.

MEA based capture seems to be a lower rate of carbon absorption, which again calls for a larger absorber column. In collaboration with Hamburg University of Technology comparative studies of the net efficiency penalty of CAP and MEA were conducted. Using modelling of the rate of absorption of carbon dioxide by aqueous ammonia and the simulation results, the dimensions of the absorber columns was estimated. An absorber about twice as high as the one used for the MEA based process was found to be required to reach 90 per cent capture using chilled ammonia.

The project was an Industrial PhD project co-supervised by Willy van Well, DONG Energy, and Erling H. Stenby, CERE.



# Thermodynamic Simulations - Learn to Love Them

While computer simulation tools are available in practically all fields of applied thermodynamics, some of the most advanced models are still not widely used by industry. A dedicated team at CERE is set on changing the scene.

n most offices at CERE you will see a white coat hanging in the corner, but Bjørn Maribo-Mogensen is an exemption to the rule. Filling a dual position as both a PhD student in thermodynamic modelling and the centre's software manager he is one of the few members of CERE's scientific staff without tasks to perform in the lab facilities.

Bjørn Maribo-

Mogensen, PhD

Manager, CERE

Student and Software

CoLAN consortium

logo. Ten years ago,

efforts to create stan-

CoLAN initiated

dards that make

CAPE Open more

accessible.

ments in thermodynamic models where he works to extend the Cubic Plus Association (CPA) equation of state to complex mixtures containing electrolytes, he is also engaged in an overall effort to make the centre's developments more accessible to industry and other partners. This is done through development of thermodynamic models that can be plugged into process simulation tools as e.g. CAPE-OPEN modules or Aspen Plus User Models. The latest achievement is a new CAPE-OPEN library which defines a simplified interface for creating CAPE-OPEN compatible modules.

"The new interface makes it possible for what I would call the average scientist - with no special insight in programming – to present his results as CAPE-OPEN modules. Obviously, the more content you'll find in the CAPE-OPEN format, the more interesting will it be to potential users in industry and at other research institution," Bjørn A high level of utilization of CAPE-OPEN is not Maribo-Mogensen says.

## The Esperanto of process simulation

CAPE-OPEN can be seen as the "Esperanto" of process simulation. The standard is a suite of protocols that enables different tools created by different companies, individuals or research in-



The CAP technique also requires use of a NH3-

A drawback of the CAP process compared to

stitutions to communicate.

The CAPE-OPEN standard is maintained by the not-for-profit CAPE-OPEN Laboratories Network (CO-LaN) consortium, which was formed in February 2001 from the Global CAPE-OPEN project. The network aims to ensure the interoperability of process simulation components.

"The basic idea is to allow for e.g. new unit operations and thermodynamics models to be shared, but without giving away source coding and other details that could be subject to confidentiality. Unfortunately, this dual purpose means that a communication platform like CAPE-OPEN can never be so simple," according to Bjørn Maribo-Mogensen.

However, it was soon realized that the first versions of the programme were just too complex. Ten years ago, the CoLAN consortium under Besides contributing to theoretical develop- the EFCE (European Federation of Chemical Engineering) initiated efforts to create standards that make CAPE Open more accessible. CERE has taken part.

> "I would say that the efforts under CoLAN have succeeded in creating CAPE-OPEN examples which are fairly simple to use as a starting point for a professional programmer. But the average researcher in either industry or academia would still have to spend a considerable amount of time learning to use it, as it requires indepth knowledge of how the CAPE-OPEN communication protocol is defined. We have succeeded in simplifying this task drastically," says Bjørn Maribo-Mogensen, adding:

> "In fact we haven't made CAPE-OPEN simpler, but the new library hides a lot of the complexity from the user."

## Gaining in predictive power

a goal in itself.

"But once more people get experience with CAPE-OPEN it will bring our other developments much closer to application. We know that industry takes great interest in this. Especially, of course, the companies that sponsor specific research programs are keen to access the results

In fact we haven't made CAPE-**OPEN** simpler, but the new library hides a lot of the complexity from the user." Bjørn Maribo-Mogensen, PhD student and software manager, CERE

and should be able to do so easily, but also others have expressed interest."

While holding a Masters degree in chemical engineering, Bjørn Maribo-Mogensen also sees himself as a programmer.

"Programming caught me in high school. Well, actually I began already in primary school, but during high school my interest took a serious turn."

At CERE's Discussion Meeting 2011, some industry representatives expressed concern over thermodynamics being left too much over to computer modelling. Computer simulations should not totally replace empirical data, they argued. Bjørn Maribo-Mogensen understands the view point:

"You still need to obtain your traditional experimental data. But I am happy to note that the predictive capability of our models is getting ever stronger. We are getting really close to what the experiments show."

## Learn to love simulations

Even the best models will not make experiments redundant, he stresses:

"We still need experimental data to verify the performance of models. But, as the models improve, we can refine the experiments so we don't need to do as many but can instead focus on getting a high quality of data from exactly the experiments we need to fill gaps."

Therefore, anybody involved in thermodynamics in either industry or academia may just as well, if not a fan already, learn to love computer simulations, according to Bjørn Maribo-Mogensen:

"The problems waiting to be solved are getting increasingly complex. If you look at oil recovery you have ever more complex conditions as you move to deeper or more remotely located fields where you need to have large amounts of hydrate inhibitors and other chemicals present in your mixtures. Then you have the whole area of carbon dioxide capture where a lot of potential solvents - ranging from amino acids to ionic liquids and many others - are available. Also a number of other problems relevant to energy production or industry processes include complex mixtures. So, as things get complex there is no way around applying simulations as one of your tools."

# PhD Defense Investigation and Modelling of **Diesel Hydrotreating Reactions**



Rasmus Risum Boesen, PhD Today works with Calsep Supervisor: Nicolas von Solms



growing number of countries have demands for ultra low sulphur diesel (ULSD). While the world's sulphur emissions have already been dramatically reduced, even small amounts of sulphur in diesel will disturb the catalyst responsible for reducing nitrogen-oxides from the exhaust gas. In other words: in order to reduce the emissions of nitrogen-oxides one needs to have ultra low sulphur content.

The project, which is carried out in collaboration with Haldor Topsøe A/S, investigates hydrotreating of diesel. Hydrotreating is an important refinery process, in which the oil stream is upgraded to meet the required environmental specifications and have the required physical properties. In a hydrotreating reactor a mixture of liquids (primarily oil) and gas (primarily hydrogen) trickle downwards through a porous catalyst. The result is sulphur bound to hydrogen in the form of H<sub>2</sub>S.

The process is complex, as the performance of the reactor is governed by intrinsic kinetics, diffusion in the pores of the catalyst, mass transfer between the phases and the equilibrium between the gas and the liquid phase.

The hydrogenation of aromatics during hydrotreating is important, as the aromatics content of the product influences the properties of the product, and

# that the Cubic Plus Association (CPA) equation of state proposed by Kontogeorgis et al. is at suitable

model for such mixtures. In the project CPA was shown to predict a

number of key factors in multi-component systems satisfactorily; i.e. methane content of liquid phase over a range of temperature and pressure. CPA was also applied to alkane + water and alkylbenzene + water systems.

Finally, CPA has been extended to reservoirfluid + MEG and reservoir-fluid + MEG + water systems. The reservoir fluid consists of three condensates and two oils from the gas fields in the North Sea. The mutual solubility of condensates and MEG was satisfactorily correlated. Similarly the mutual solubility of condensate/oil, MEG and water was predicted satisfactorily. Also the experimental trends in mutual solubility as a function of the temperature and MEG content in polar phase was predicted satisfactorily.



Mohammad Riaz, PhD Supervisor: Georgios Kontogeorgis



PhD Defense **Distribution of Complex** Chemicals in Oil-Water Systems

Deep water oil and gas exploration and produ-ction have increased significantly in recent years. Production at deep water involves a number of challenges. For instance, the deepwater environment exposes the flow lines to temperatures near 4 degrees C, which can create production problems in sub-sea flow and pipework due to formation of gas hydrates. These hydrate plugs have been known to form as long as 6.2 miles and have blocked pipelines up till 40 inches in diameter. In order to inhibit gas hydrate formation monoethylene glycol (MEG) and methanol are injected in large amounts.

The purpose of this project is to map the distribution of these complex chemicals in oil-water systems through a combination of experimental measurements and thermodynamic modelling. It is important to know the distribution of these chemicals in oil and water systems for economical operation of a production facility and to evaluate their impact on marine life; while this information is also of

value for downstream processing of oil and gas.

In order to develop a thermodynamic model for this purpose, experimental data are required. However such data with natural gas-condensate / oil systems are very rare in literature. In this project experimental work has been carried out at Statoil Research Center in Norway.

The mutual solubility of two North Sea condensates, MEG and water has been measured in the temperature range of 275-326 K at atmospheric pressure. The detailed composition of condensates was measured by GC analysis and 85 components are identified up to n-nonane and hundreds of ill-defined components in decane plus fraction.

The systems of water, hydrocarbons and chemicals represent complex mixtures containing associating polar and non-associating compounds. Widely used equations of state in the oil and gas industry such as SRK and PR cannot describe such systems satisfactorily. It has been shown previously

Wells

since the conversion is important for the hydrogen consumption. It is well-known that saturation of fused aromatic rings can be limited by thermodynamic equilibrium at typical industrial hydrotreating conditions. Equilibrium constants have been calculated based on experimental measurements for the hydrogenation of naphthalene and phenanthrene.

Feeds used in the hydrotreating process are complex mixtures with a large number of compounds. In this work a model-diesel feed consisting of 13 compounds, representing the most important component classes, has been hydrotreated on a commercial NiMo catalyst. The difference in reactivity and behaviour of the different compounds has been investigated.

A steady-state trickle-bed reactor model has been set up. The heterogeneous model considers co-current flow of two fluid phases, gas and liquid. As reactor models are becoming an important tool to understand the process, detailed kinetics models are needed. So called Robinson-Mahoney reactors allow for direct measurement of reaction rates and can thus be used to develop kinetic models. A reactor model for a Robinson-Mahoney reactor that takes mass transfer into account is presented, and it has been used to test a set of kinetic models at industrial conditions.



# A Companion for **History Matching**



CERE's geophysics group has produced a computational tool for finding the geological structure of an oil and gas reservoir; a task previously not possible within practical time frames.

Known as history matching, the traditional method for modelling the permeability structure of an oil and gas reservoir by use of data from production is to have your computer search for known reservoir models that match the data observed. While history matching will continue to be a valuable tool for industry and academia, the geophysics group at CERE has succeeded in developing an alternative method.

"History matching is not the ideal tool because the solutions you get will typically not resemble the true geological structure. For instance they will neither have the characteristic geological layers, nor the channels known from real geology. Instead such features are hidden or averaged out. Further, history matching most often results in two or more different solutions that could match the oil production observed," says Professor Klaus Mosegaard, head of the group, adding:

applied within acceptable time frames have developed," Klaus Mosegaard concludes.

previously not been available as they have been too demanding in terms of computer resources."

In the alternative approach, firstly the group will find a reservoir model which is known to structure known to have some resemblance to the reservoir which is *exist in the reservoir* to be investigated. Secondly, a geology expert will elaborate the model into a sketch of the basic type of structure that can be imagined for the reservoir *a hypothetical reser*in question (illustration A).

"We are aware that the real reservoir from dominant geological which we have data from actual production will not look like this model. However, we do know that certain key features will be right; in the example first of all the way that the two dominant geological materials are arranged in the characteristic winding patterns," Klaus Mosegaard explains.

"So, when we have our computer search for possible matches to the production data – much like it would do in traditional history matching - we have inserted an algorithm which only allows for solutions, which resemble the sketched structure."

An illustration of a solution is shown in illustration B. Finally, illustration C shows calculated oil saturation in the reservoir at a given moment. in the reservoir at a gi-

"To our knowledge this is the first time an algorithm allowing this type of calculation within "However, alternative methods that can be a practically acceptable time horizon has been

*In the new method*, firstly a geology expert will sketch the type of (A). In the example is shown a structure for voir with two types of material; the darker areas have high permeability, the brighter have low permeability. The computer will then search for solutions that match data from production, but only allowing a solution that agree with the sketch's features. A solution is shown in (B). Finally (C) shows calculated oil saturation ven moment.

Wei Yan,

Senior Scientist, CERE

I am convinced

**7** that the tools

we develop are of

genuine interest

to a large number

of engineers who

need accurate de-

scriptions of phase

equilibria and other

in their daily work.

Senior Scientist

Wei Yan, CERE

important properties



# Mandarin Speaking Senior Scientist

Having worked with the Center since 2001, Wei Yan fills a new strategically important position at CERE.

ronferences with joint participation from industry and academia often display some friendly teasing between the two groups, but when some industry representatives at CERE's Discussion Meeting 2011 voiced mild frustrations over certain thermodynamic models being at DTU and accepted. too complex and heavy in regard to computer resources, one of the Centers' researchers almost jumped up from his chair to take the floor. To Wei Yan this topic is very close to heart.

"It is my dream to bridge the models we create with the needs of industry. I am really convinced at CERE has existed for 30 years. This is quite that the tools we develop are of genuine interest to a large number of engineers who need accurate descriptions of phase equilibria and other important properties in their daily work," Wei transfer between generations of scientists is Yan says.

"We have to realize, though, that we often need to simplify our models if we want them to be applicable to industry. But at the same time we also want our models to give their descriptions as accurately as possible. There isn't a simple solution to this dilemma. It is very challenging and it is something we have to think about and improve constantly."

## Looking forward to further collaboration with China

Wei Yan still feels well connected to his country of birth and speaks mandarin with a Beijing dialect, in which his countrymen - at least according to himself! - are not able to sense that he has spent a decade abroad.

Obviously he is also part of the ongoing collaboration between CERE and the University of Petroleum in Beijing and other Chinese institutions. A collaboration which has gained further strength as China Petro-



## A position of strategic importance

During his PhD-studies at the University of Petroleum in Beijing, China from 1996, Wei Yan took interest in works by the thermodynamics group at DTU around the UNIFAC model and stability analysis for flash calculation. After obtaining his degree from the university in Beijing in 1999, he employed at the university as a teacher, but kept in contact with the centre at DTU. In 2001 he was offered a post doc position

"I was attracted by the fact that CERE on the one hand has a very high scientific level but on the other hand also has strong commitment to its research being application oriented," he recalls.

"The research group around thermodynamics mature for this field, and we have easy access to all publications made during the centre's entire existence. This is a major stronghold. Also the running smoothly."

After his post doc Wei Yan worked as researcher in various CERE projects. Now he has been employed in a newly created position as senior scientist in CERE at DTU Chemistry. The position is of strategic importance to CERE and will allow him to use his broad experiences both in experimental and theoretical thermodynamics to contribute to different scientific areas in the Center.

leum & Chemical Corporation – or Sinopec Corp - joined CERE's industry Consortium in 2009.

"I had the opportunity to visit their laboratories in Beijing recently, and I was impressed by the scale of investments they are making. They are upgrading their equipment very fast and I am looking forward to finding ways to set up further collaboration," Wei Yan comments.



"In my new capacity, I will be less dependent on the time frames of individual projects. It will give me more flexibility and more scope to pursue my own ideas," he states.

## Improving the speed of calculations

As thermodynamic modelling is an integrated part of most activities at CERE, Wei Yan plays a role in many projects. For instance, he is the prime responsible for the centre's engagement in CompSim, which is a project dedicated to compositional reservoir simulation:

"This is of course not a new topic. To describe the strong compositional effects in reservoir processes like gas injection, an accurate compositional model is required. Meanwhile, we would like to improve the speed of calculations with the more complicated fluid model. It requires an integrated effort on models, algorithms, and implementations."

"The efficient flash algorithms developed in CERE form the basis of our study. By allowing approximation to a certain extent, the simulation speed can be further improved. The method can also be applied to more complicated thermodynamic models. I hope we will be able to attract more attention to our methods and to persuade industry to integrate them. I am convinced they can be of great value to many engineers out there."

The thermodynamic models produced at CERE will often need to be simplified in order to be applicable to industry. But at the same time the models need to give their descriptions as accurately as possible. There is no simple solution to this dilemma.



of Chevron visited CERE to present a highly interesting CO<sub>2</sub> injection case.

# At a well attended ses-sion, Dr. Dengen Zhou A Chevron View at Carbon Dioxide Flooding

found carbon dioxide flooding to be a surprisingly efficient EOR method in dense chalk. Denmark, and the centre was pleased to host a seminar at October 4th 2011, where Dr. Dengen Zhou of Chevron Energy Technology Company presented US carbon dioxide flooding experiences.

Since 2010, Dengen Zhou has led Chevron's CO2 Center of Excellence. From 2007 to 2010, he serviced as Engineering Technical Team Leader in Mid-Continent/Alaska (MCA) Business Unit, responsible for design and optimization of CO<sub>2</sub> flood EOR projects. Before he started working on CO<sub>2</sub> projects, Dengen Zhou was the subsurface coordinator for a heavy oil development project in Bohai Bay, China for four years, representing Chevron's interests through all project phases from design, to implementation, to production. Dengen Zhou started his Chevron career as a consulting engineer and worked on a wide range of recovery optimization projects: waterflood optimization, gas production and storage and miscible gas injection. He holds a BS degree in Chemical Engineering from the China University recovery efficiency.

n 2010, Danish studies coordinated by CERE of Petroleum, and a PhD degree in Chemical Engineering from DTU.

Dr. Zhou presented a CO<sub>2</sub> injection case This has raised awareness to the method in history from Reinecke field located in the Pennsylvanian Canyon Reef trend in West Texas. The field consists of two main parts; a southern structural dome (South Dome) and a northwest region. The South Dome has been CO<sub>2</sub> flooded for about 10 years using a gravity-stable/straight CO<sub>2</sub> design.

> Ten-year's production data from the field suggests a limited success of the gravity-stable design with excellent initial CO<sub>2</sub> incremental responses but significant operational and reservoir management challenges as the injection matures. Comparison of the design concept and the actual field performance reveals the key gaps in this original design. Field performance and geological characterization suggest that CO<sub>2</sub> channels through high permeability conduits and short-circuits the original gravity stable design, which lead to high gas recycling and high CO<sub>2</sub> utilization factor. An optimization plan is proposed to convert continuous CO<sub>2</sub> injection to WAG to improve the field operability and field

# New Faculty Member An Entrepreneur and a Scientist

**O**riginally writing both his Master Thesis and PhD Thesis within chemical engineering, Associate Professor John Bagterp Jørgensen has spent most of his career as a computer modelling specialist. Over recent years his interest has returned to its starting point as several applications of his work within predictive computational models have proven relevant to chemical engineering. These include optimization of oil recovery and modelling of smart energy systems capable of integrating large amounts of highly variable, renewable energy sources.

Shortly after completion of his PhD, John Bagterp Jørgensen was engaged in a start-up company delivering predictive computational models for specific industry purposes. A number of major Danish industries were among its clients. However, he decided to resume his academic career and was offered a position as associate professor at DTU Informatics.

Through the Joint Industry Project ADORE, coordinated by CERE, John Bagterp Jørgensen has worked with members of the CERE Industry Consortium on predictive computational models aimed at optimization of oil recovery. With the recent broadening of CERE's general scope to include a range of energy technologies, also cooperation with other CERE faculty on models for smart energy systems has become relevant.



Thus, it was natural for John Bagterp Jørgensen to become a CERE faculty member by May 2011.

The position is dual meaning that he is both a member of the CERE Faculty and of the Faculty of DTU Informatics.

# Two new Professors at CERE



da L. Fabricius was appointed Professor in Petroleum Engineering Geology at DTU Civil Engineering as of September 1st 2011. She holds a M.Sc. degree in geology (mineralogy) as well as PhD and Dr.Techn. degrees in applied geology. After completing her M.Sc. degree, she worked a few years as a petroleum geologist before joining DTU. Her research includes integration of rock mechanical, geophysical and geological information. It has until recently mainly focused on chalk, but now includes

other sedimentary rocks as sandstone, shale and diatomite.

In 2011, two CERE faculty members were appointed Professors.

eorgios Kontogeorgis was appointed Professor in Chemical and Bioche-Umical Engineering Thermodynamics at DTU Chemical Engineering as of February 1st 2011. He holds a M.Sc. degree in chemical engineering from the Technical University of Athens, Greece (1991), and a PhD degree from DTU (1995). He joined DTU as Associate Professor in 1999. His fields of interest range from energy (mainly thermodynamic models for oil and gas applications) over materials science and nanotechnology (especially polymers) to environment and recently also biotechnology.





# Danish PetroChallenge Winners

team from the Danish high school CELF competition is organized by CERE. In all coun-**M**HTX, Nykøbing Falster, won not only the Danish version of the international PetroChallenge competition 2011, but also the international final held in London.

All classes participating in the PetroChallenge competition are invited to visit CERE where demonstrations of the Centre's equipment are given.

Since its introduction in 2005, the Danish version of the PetroChallenge competition has steadily attracted a growing number of high schools, setting a new record for participation each year. 1,250 students from 30 high schools engaged in the competition's virtual hunt for undiscovered offshore oil reserves in 2011. The Danish branch of the PetroChallenge



tries involved, students use the OilSim simulation tool developed by Simprentis - a tool also applied in real oil discovery.

During the competition the various phases of oil discovery are simulated. Including one realistic feature - with every step forward your costs accelerate.

The 2011 version of the Danish PetroChallenge competition was sponsored by Maersk Oil and DONG Energy. All participating classes are invited to visit CERE and several do so.



# A Summit of Energy Engineering

International industry participation reached a new peak at CERE's Discussion Meeting 2011.

With 35 external participants representing 20 companies from 13 countries, the 2011 version of CERE's Discussion Meeting set a new record in industry participation. The annual

event is where the centre's industrial Consortium – counting more than thirty international and Danish member companies with interests within energy, pharmacy and chemistry – join CERE researchers to share experiences and exchange ideas. Please join us for a tour of the event held from June 8th – June 10th 2011 at Pharmakon conference centre, Hillerød.

I come here because CERE is actively engaged in finding real solutions to industrial problems," says Dr. Susan Little, Senior Chemist at BP. "Part of my role is to disseminate information on new and evolving technologies to my colleagues and every year I am able to do so."



search portfolio to develop technologies and knowledge that can further maximise the efficient production of oil and gas from the fields we operate," says Nigel Jenvey, Director of EOR at Maersk Oil. "The Discussion Meeting is a good example of the merits of such cooperative efforts. Through bringing industry and academia together to meet students, network together and review and plan work will ultimately give the greatest chance of solving the most important problems to the benefit of all participants and ultimately society at large."

CERE forms a key part of our global re-



Dr. Bret Beckner of Exxon-Mobil was one of the new faces at the 2011 meeting: "I would say that chances of us returning next year are good. The conference offers a comprehensive review of the science presented and you have an opportunity for going into depth with the issues.



I like to get an impression of where the centre is heading. It is interesting to see how a topic grows over the years," says Dr. Oliver Koch of Linde – present at his 9th Discussion Meeting. "Had I not missed one year, this would have been my 10th anniversary! The event is my chance to influence the direction of the centre's research. Also, it is a nice opportunity to establish contacts with other indu



Also, it is a nice opportunity to establish contacts with other industry representatives."



Sinopec of China joined the CERE industrial Consortium in 2009. The company, today one of the world's largest energy corporations, maintained a strong presence at the 2011 event with five representatives. According to Dr. Zengmin Lun of Sinopec research centre PE-PRIS in Beijing especially CERE's work within carbon capture and storage (CCS) is of interest to his centre, as China currently has ambitious plans for CCS with several demonstration projects ongoing. His colleague Dr. Yingchen Li (picture) of Sinopec research centre SRIPT in Shanghai is focussing on CERE's research within Enhanced Oil Recovery (EOR).



It is a great pleasure to be able to discuss in depth with others that share the same interest – all of my everyday colleagues at home are either reservoir engineers or chemists," says Dr. Klaus Potsch of Austrian based oil corporation OMV - coming from a background as a physicist with a PhD in fluid dynamics. "I simply cannot find time in my working day to get the results that come from projects like CERE's. So it is of great value for me to come here and pick up on the latest developments."



Erling Stenby Chairman of CERE Professor ehst@kemi.dtu.dk

# Keeping up the Pace

After last years' "jump start" in our first year as CERE, 2011 saw a further rise in activity and also an expansion of our faculty.

n my introduction to last years' annual report I referred to CERE's first year, 2010, as "a jump start". Fortunately, we have by no means lost pace since. Much to the contrary, we were able to launch some of the largest projects in the centre's history during 2011.

The SmartWater project will study chemically modified water as an easily accessible and sustainable method for enhanced oil recovery. The project is funded for a four-year period by the EUDP program (under the Danish Ministry cius. of Climate and Energy), Maersk Oil and DONG Energy.

The BioRec project (Biotechnology in Oil Recovery) is a unique partnership between oil industry - represented by Maersk Oil and DONG Energy - and biotechnology, represented by Novozymes. This is a four-year project funded by The Danish National Advanced Technology Foundation, Maersk Oil and DONG Energy.

Thirdly, the new project "CO2 Hydrates -Challenges and possibilities" is a collaboration between Professor Georgios Kontogeorgis and Ecole des Mines in France. The project received funding from the Danish Council for Independent Research in close competition.

In addition, a new project sponsored by the European gas industry the GERG organization was launched in 2011. This project addresses the challenges of accurate predictions of dew point in natural gas within varying content of water.

Another rapidly growing activity is research concerning post-combustion CO<sub>2</sub>-capture. Within this area the centre is involved in several projects and extensive EU collaborations.

## A larger, stronger faculty

In 2011 we were able to congratulate two CERE faculty members with their new titles as Professors - Georgios Kontogeorgis and Ida L. Fabri-

Also, we were able to welcome two new faculty members; Associate Professor John Bagterp Jørgensen and Assistant Professor Philip Fosbøl.

John Bagterp Jørgensen has a background which is highly interesting in relation to CERE. Not only is he a chemical engineer with a computer modelling specialization; he also has extensive entrepreneurship experience thus allowing him to easily see things from an industry point of view when engaging in joint projects. His projects include predictive computational models relevant





to optimization of oil recovery and modelling of smart energy systems capable of integrating large amounts of highly variable, renewable energy Professor Georgios Kontogeorgis. The course, resources.

CERE for some time. By integrating laboratory experiments and computer modelling smoothly in his works, he symbolizes what the Center as such does best. In recent years carbon capture has occupied a significant proportion of his efforts, and we expect that he will further strengthen our engagement in this field in his new capacity.

In addition, I am pleased to note that Wei Yan - who has been with us since 2001 - has accepted a newly created position as Senior Scientist. The position will allow him to use his broad experiences both in experimental and different scientific areas in the Center.

## Yet another successful summer school

The 2011 CERE annual Discussion Meeting was, as always, a very interesting and inspiring meeting. With the 35 external participants representing 20 companies form 13 countries, the 2011 meeting set a new record in industry participation.

Another reoccurring event was the advanced summer school within thermodynamics by Professor Michael L. Michelsen - the "Advan-





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ced Course on Thermodynamic Models: Fundamentals & Computational Aspects" - with held in August, was, as always, a great success Philip Fosbøl has been a key scientist at and extremely well attended, not least by industry participants.

> Also, we are proud to announce that the 2011 Christopher J. Wormald prize was presented to a PhD student in the Center, Ane Avlund, during the Thermodynamics 2011 conference in Athens in August 2011, for her innovative research in thermodynamics. Ane Avlund graduated in 2011.

Finally, I would like to mention that Danish version of the international PetroChallenge competition 2011, coordinated by CERE, set a new record for participation with 1,250 students from 30 high schools attending. We see the comtheoretical thermodynamics to contribute to petition as one of the ways to secure our supply chain in terms of future engineering students. Over the years many students have benefited from the close contact with Danish and international industry through a project in CERE, and I have every reason to believe that this will continue to be the case.

> If any of the above sparks a special interest or calls for further investigation, you are as always welcome to contact me.

# **Research funding**

management bonuses nor investor dividends are due, and gradually all funding received will be invested with the aim of maximizing the production of high quality research results and

As a university research center our objective highly skilled researchers at PhD and post doc level.

The research carried out in CERE is funded by grants from a number of public and private sponsors. During 2011 our external funding increased significantly to a total budget of EUR 4.6 million.

## **Research Funding**

The external funding received in 2011 fell under the following projects and categories (all amounts in kEUR):

CHIGP	594
ADORE	580
CO2 EOR	243
CCS	432
GAS HYDRATES	405
PhD DTU	202
BIOREC	297
SMART WATER	175
HEHO	94
ROCK PHYSICS	189
IMGP*	503
other private	797
other public	94





# Conference contributions & Invited speakers

Ahsan, R.; Fabricius, I.L. 2010: "Sorption of Magnesium and Sulfate lons on Calcite" (Poster presentation), In: A new spring for geoscience: 72nd EAGE conference and exhibition, Barce-Iona 14-17 June 2010 ; Conference proceedings & exhibitors' catalogue. CD-ROM / Editor - DB Houten, NL : EAGE, 2010.

Alam, M.M.; Akam, H. N.; Fabricius, I.L.; 2011 "Effect of fluid-solid friction on the stiffness of chalk", (Poster presentation), 1st International Workshop on Rock Physics, Colorado School of Mines, Golden, Colorado USA

Alam, M.M.; Hjuler, M.L.; Christensen, H.F.; Foged, H.; Fabricius, I.L.; 2011 "Impact of supercritical CO<sub>2</sub> injection on petrophysical and rock mechanics properties of chalk: an experimental study on chalk from South Arne field, North Sea", (Oral presentation), SPE Annual Technical Conference and Exhibition. Denver, Colorado, USA, SPE 14056

Monzurul Alam, M.; Niu, B.; Fabricius, I.L.; Yan, W.; Shapiro, A.A.; Stenby, E.H.; Christensen, H.F.; Ditlevsen, F.P.; Hjuler, M.L.; Olsen, D.; 2011 "Enhanced Oil Recovery Through CO<sub>2</sub> Utilization" (Poster presentation), SPE Forum - CO<sub>2</sub> Geological Storage: Will We Be Ready in Time? The Algarve, Portugal

Avlund, Ane; Kontogeorgis, Georgios, M.; Michelsen, Michael, L.; 2011 "Modeling of glycol ethers with sPC-SAFT", (Invited speaker), Thermodynamics 2011, Athens, Greece





Belkadi, Abdelkrim; Yan, Wei; Michelsen, Michael L.; Stenby, Erling H.; 2011 "Comparison of Two Methods for Speeding up Flash Calculations in Compositional Simulations", (Invited speaker), SPE Reservoir Simulation Symposium, The Woodlands, Texas, USA, SPE 142132

Darde, Victor; Well, Willy J.M. van; Stenby, Erling H. Stenby; Thomsen, Kaj; 2011 "CO<sub>2</sub> capture using aqueous ammonia: kinetic study and process simulation", (Oral), GHGT10 conference, Amsterdam, The Netherlands, September 2010, Journal Energy Procedia, 4 (2011) 1443-1450

Diaz Tovar, Carlos Axel; Mustaffa, Azizul Azri; Kontogeorgis, Georgios; Gani, Rafiqul; Sarup, Bent; 2011: "Lipid Processing Technology: Shifting From Waste Streams to High-Value Commercial by-Products" . (Oral presentation), AICHE American Congress of Chemical Engineering . Minneapolis, MN, USA

Fabricius, I.L.; 2011 "Relationship between elastic moduli and pore radius in clay aggregates", (Poster presentation), Unconventional ressources and the role of technology. 73rd EAGE Conferenc & exhibition, Vienna, Austria, CD-ROM, Article no. P307

Fabricius, I.L.; Eberli, G.P.; 2011 "Sonic velocitirs in carbonates. "Shear weakening" is better described as "air stiffening" (Poster presentation), 14th Bathurst Meeting of Carbonate Sedimentologists, University of Bristol





Fabricius, I.L.; 2011 "Pore fluid effect on chalk and clay elasticity" (Invited speaker), Frontiers in diagenesis: Clay & Carbonate facies and their diagenetic pathways in reservoir rocks. Cambridge, (Mineralogical Society)

Fabricius, I.L.; 2011 "High kinemstic viscosity of air may cause dry clay to be stiffer than water saturated clay", (Oral presentation), 9th Euroconference on Rock Physics and Geomechanics, Trondheim, Norway, Abstracts 176-177

Fosbøl, Philip L.; Thomsen, Kaj; 2011 "Absorption and Desorption Modelling United", (Oral presentation), ICEPE, Efficient Carbon Capture for Coal Power Plants, Frankfurt am Main, Germany

Fosbøl, Philip Loldrup; 2011 "Post Combustion CCS activities at Center for Energy Resources Engineering", (Oral presentation), DTU Climate Centre Seminar on CCS, DTU Chemical Engineering, DTU, Kgs. Lyngby, Denmark

Hendriks, E.; Kontogeorgis, G.M.; Dohrn, R.; De Hemptinne, J.-C.; Economou, I.; Fele Zilnik, L.; Vesovic, V.; 2011 "Industrial Requirements for Thermodynamics and Transport Properties - Before and Now", (Oral presentation), 25th European Symposium on Applied Thermodynamics, ESAT 2011, Saint Petersburg, Russia

Herslund, Peter Jørgensen; Solms, Nicolas von; Thomsen, Kaj; Abildskov, Jens; 2011 "Thermodynamic Modeling of Gas Hydrate Forming Systems Including Thermodynamic Promoters for a Novel CO2 Capture Process", (Poster presentation), the 7th International Conference on Gas Hydrates (ICGH 2011), Edinburgh, Scotland, United Kingdom

Hossain, Z; Fabricius, I.L.; 2011 "CO2 injection effect on physical properties of greensand from the North Sea" (Oral presentation), Unconventional ressources and the role of technology, 73rd EAGE Conferenc & exhibition, Vienna, Austria, CD-ROM, Article no. D017, 2011

Hossain, Z.; Mukerji, T.; Fabricius, I.L.; 2011 "Biot's and squirt flow mechanism of greensand as interpreted using NMR data", (Poster presentation), 1st International Workshop on Rock Physics, Colorado School of Mines, Golden, Colorado USA

Hossain, Z.; Mukerji, T.; Fabricius, I.L.; 2011 "Influence of pore fluid and frequency on elastic properties of greensand as interpreted using NMR data", (Oral presentation), SEG San Antonio Annual Meeting 2011, Abstracts 2177-2182

Jensen, Lars; Ramløv, Hans; Thomsen, Kaj; Solms, Nicolas von; 2011 "Inhibition of gas hydrate formation by low-dosage, environmentally benign inhibitors", (Oral presentation), Proceedings of the 2nd annual Gas Processing Symposium, Doha, Qatar, 2011 (ISBN: 0444535888)

Jørgensen, John Bagterp; Huusom, Jakob Kjøbsted; Rawlings, James B.; 2011 "Finite Horizon MPC for Systems in Innovation Form" (Oral presentation), Proceeding of the 50th IEEE Conference on Decision and Control and European Control Conference . Orlando, Florida, USA

Kontogeorgis, Georgios; Tsivintzelis, Ioannis; Stenby, Erling H.; 2011 "Chemicals in Gas Processing (CHIGP): An industrial project for the thermodynamics of complex petroleum fluids and chemicals" (Oral presentation), 19th

European Conference on Thermophysical Properties, Thessaloniki, Greece

Kontogeorgis, Georgios; Economou, Ioannis, G.; Maribo-Mogensen, Bjørn; Kontogeorgis, Georgios M.; Thomsen, Kaj; 2011 "An Electrolyte CPA Coutsikos, Philippos; 2011 "On the true value of cubic equations of state", (Oral presentation), Equation of State for Applications in the Oil and Thermodynamics 2011, Athens, Greece Gas Industry" (Poster presentation), the SAFT 2011 Workshop, Pau, France,

Kontogeorgis, Georgios; Tsivintzelis, Ioannis; Riaz, Muhammad; Michelsen, Michael, L.; Stenby, Erling H.; 2011 "Recent applications of the CPA Equation of State for the petroleum industry", (Poster presentation), SAFT2011, Pau, France

Lange, Katrine; Cordua, Knud Skou; Frydendall, Jan; Hansen, Thomas Mejer; Mosegaard, Klaus; 2011 "A Frequency Matching Method for Generation of a Priori Sample Models from Training Images", (Oral presentation), Proceedings of IAMG 2011 - Annual Conference of the International Association for Mathematical Geosciences

Mbia, E.N.; Fabricius, I.L.; Oji, C.O.; 2011 "Petrophysics of shale intervals in the Skjold Field, Danish North Sea" (Oral presentation), Unconventional ressources and the role of technology, 73rd EAGE Conferenc & exhibition, Vienna, Austria, CD-ROM, Article no. D018, 2011

Maribo-Mogensen, Bjørn; Kontogeorgis, Georgios M.; Thomsen , Kaj; 2011 "An Electrolyte CPA Equation of State for Applications in the Oil and Gas Industry", (Poster presentation), the Riaz, Muhammad; Kontogeorgis, G.M.; Stenby, 25th European Symposium of Applied Thermodynamics (ESAT), St. Petersburg, Russia

Maribo-Mogensen, Bjørn; Kontogeorgis, Georgios M.; Thomsen, Kaj; 2011 "Development of a CAPE-OPEN compatible library for thermodynamic models and unit operations using .NET"







(Oral presentation), the 8th European Congress of Chemical Engineering, Berlin, Germany

Mosegaard, K., Melnikova, Y., Lange K., Cordua, K., Frydendall, J., and Hansen, T. M.; 2011 "Sharper images of reservoir structure - A geostatistical approach to data inversion", (Oral presentation), 32nd Annual IEA EOR Symposium and Workshop, Vienna, 17 to 19 October 2011.

Mosegaard, K.; 2011 "Geophysical inversion constrained by model prototypes", (Invited speaker), ETH, Zürich, 16. September 2011.

Mosegaard, K.; 2011 "On Frequency Matching and the Explicit Calculation of Prior Probabilities from Training Images", (Poster presentation), IAMG 2011, Salzburg.

Musko, N.E.; Kontogeorgis, G.M.; Grunwaldt, J.-D.; Tsivintzelis I.; 2011 "Phase Behaviour Modelling of Chemical Reactions in Dense and Supercritical Carbon Dioxide using the Cubic-Plus-Association Equation of State", (Poster presentation), The 25th European Symposium of Applied Thermodynamics, Saint Petersburg, Russia

E.H.; Yan, W.; Haugum, T.; Christensen, K.O.; Solbraa, E.; Løkken, T.V.; 2011 "Distribution of gas hydrate inhibitors in oil and gas production systems", (Oral presentation), 25th European Symposium on Applied Thermodynamics, ESAT 2011, Saint Petersburg, Russia





Sadegh, Negar; Kontogeorgis, Georgios; Stenby, Erling Halfdan; Thomsen, Kaj; 2011 "Thermodynamic modeling of sour gas cleaning process with alkanolamine", (Oral presentation), 25th European symposium on Applied Thermodynamics, ESAT 2011, Saint Petersburg, Russia

Sandersen, Sara Bülow; Stenby, Erling H.; Solms, Nicolas von; 2011 "Pressure Effect on Phase Behavior of Surfactant System", (Poster presentation), 25th European Symposium on Applied Thermodynamics, ESAT 2011, Saint Petersburg, Russia

Sandersen, Sara Bülow; Stenby, Erling H.; Solms, Nicolas von; 2011 "Phase Behavior in EOR Surfactant Flooding", (Poster presentation), Thermodynamics 2011, Athens, Greece

Sørensen, M.K.; Fabricius, I.L.; 2011 "Elastic moduli of sandstones saturated with a range of pore fluids correlated with kinematic viscosity and frequency ratio", (Poster presentation), SEG San Antonio Annual Meeting 2011, Abstracts 2297-2301

Thomsen, Kaj; 2011 "Current status of R&D in post combustion CO2 capture", (Invited speaker), Chalmers Energy Conference, Chalmers Campus, Göteborg, Sverige

Thomsen, Kaj; 2011 "Phase Equilibrium in Amino Acid Salt Systems for CO<sub>2</sub> Capture", (Invited speaker), Gassonova, Norway

Thomsen, Kaj; 2011 "Chemical Absorption Materials for CO<sub>2</sub> Capture", (Invited speaker) ICEPE 2, Second International Conference on Energy Process Engineering, DECHEMA-Haus, Frankfurt am Main, Germany

Tsivintzelis, Ioannis; Beier, Matthias; Grunwaldt, Jan-Dierk; Kontogeorgis, Georgios M.;

2011 "Phase equilibria of mixtures related to the catalytic oxidation of alcohols in supercritical CO<sub>2</sub>: An experimental and theoretical study" (Poster presentation), 19th European conference on Thermophysical Properties (19th ECTP), Thessaloniki, Greece

Tsivintzelis, I.; Kontogeorgis, G.M.; Michelsen,

M.; Stenby, E.H.; 2011 "Modeling of Mixtures with Acid Gases using the CPA Equation of State", (Poster presention), The 25th European Symposium of Applied Thermodynamics, Saint Petersburg, Russia

Tsivintzelis, Ioannis; Michelsen, Michael L.; Stenby, Erling H.; Kontogeorgis, Georgios M.; 2011 "Modeling of Mixtures with Acid Gases using CPA", (Poster presentation) Proceedings of the Thermodynamics 2011 conference, Athens, Greece.

Tsivintzelis, Ioannis; Kontogeorgis, Georgios M.; 2011 "On the Complex Hydrogen Bonding Behavior of Organic Acids", (Oral presentation), Proceedings of the 8th Hellenic Conference of Chemical Engineering, Thessaloniki, Greece

Völcker, Carsten; Jørgensen, John Bagterp; Stenby, Erling Halfdan; 2011 "Oil Reservoir Production Optimization using Optimal Control", (Oral presentation), 50th IEEE Conference on Decision and Control and European Control Conference, 2011 50th IEEE Conference on Decision and Control and European Control Conference

Waseem Arshad, Muhammad; Thomsen, Kaj; 2011 "Freezing Point Depression of Aqueous Solutions of DEEA, MAPA and DEEA-MAPA with and without CO<sub>2</sub> Loading" (Oral presentation),

ICEPE, Efficient Carbon Capture for Coal Power Plants, Frankfurt am Main, Germany

Yan, Wei; Langlais, C.; Stenby, E.H.; 2011 "Viscosity modelling of alcohols using the CPA EoS and the friction theory", (Poster presentation), 19th European Conference on Thermophysical Properties, 19th ECTP, Thessaloniki, Greece

## Yan, Wei; Michelsen, Michael L.; Stenby, Erling

H.; 2011 "Two Practical Aspects of Compositional Reservoir Simulations with PC-SAFT", (Poster presentation), SAFT2011, Pau, France

Yan, W.; Michelsen, M.L., Stenby, E.H.; 2011 "Non-Cubic EoS for Reservoir Simulations: Computation Time and PVT Modelling" (Poster presentation), SPE Applied Technology Workshop Complex Reservoir Fluids-New Developments and Multi-Discipline Integration, Amsterdam, The Netherlands

Yan, W.; Michelsen, M.L.; Stenby, E.H.; 2011 "On Application of Non-cubic EoS to Compositional Reservoir Simulation" (Oral presentation), the SPE EUROPEC/EAGE Annual Conference and Exhibition held in Vienna, Austria, SPE 142995

Yan, W.; Michelsen, M.L.; Stenby, E.H.; Belkadi,

A.: 2011 "On Two Flash Methods for Compositional Reservoir Simulations: Table Look-up and Reduced Variables" (Oral presentation), the 32nd Annual Symposium and Workshop for the IEA Collaborative Project on Enhanced Oil Recovery, Vienna, Austria.

Yuan, Hao; Shapiro, Alexander; 2011 "Filtration in Porous Media : Influential Parameters and Comparison with Experiments" (Poster presentation), Third International Conference on Porous Media . Bordeaux, France

Yuan, Hao; Shapiro, Alexander; Stenby, Erling Halfdan; 2011 "Physical mechanisms of deep bed filtration with application to the problems of petroleum industry" (Oral presentation), 2011 Bit's 2nd Annual World Congress of Well Stimulation and EOR, Chongqing, China

Zahid, Adeel; Sandersen, Sara Bülow; Shapiro, Alexander; Solms, Nicolas von; Stenby, Erling H.; Yuan, Hao; 2011 "Advanced Waterflooding in Chalk Reservoirs: Crude Oil/Brine Interaction Study", (Oral presentation), Bit's 2nd Annual World Congress of Well Stimulation and EOR, Chongging, China

# Master Thesis 2011

Shahid Ali "Application of the CPA EoS to CO<sub>2</sub> mixtures"

## Pernille Damgaard

"Assessment of electrostatics involved in polyelectrolyte adsorption onto surfaces via zeta potential technology"

Erin de Haas "Gas diffusivity in heavy oil and its influence on foamy oil behavior"

Janusz Karol Jektvik "Water conformance in horizontal wells"

Thomas Uffelmann Mohn "Effect of the salinity of the injection water on oil recovery"

Wiktor Tomasz Musialski "Rock physical modeling of greensand"

Peter Sommer-Larsen "Porosity preservation effects in chalk"

Hans Jerik Folmer Thøgersen "Effect of the salinity of the injection water on oil recovery"

**Mustafe Ahmed Yussuf** "Measurement of Phase Equilibria for Oil-Water-MEG Mixtures"

Elena Kolster "Impact cratering mechanics"

Allan Bo Hansen "Coupled Inversion of Cross Borehole Georader and Gravity Measurements"

Daniel Bo Christiansen "Monte Carlo Inversion of seismic reflection amplitudes"

**Rasmus** Juncher "Seismic amplitude reflections- A litterature study in AVO analysis"

Andreas Rosing "Tomographic Inversion of Lg Surface Waves in Norehern Europa"

# Publications 2011

Previously submitted manuscripts, published in 2011

SEP 0916 "Modelling of Phase Equilibria with CPA using the Homomorph Approach"

 Martin P. Breil, Ioannis Tsivintzelis, and Georgios M. Kontogeorgis

(Fluid Phase Equilibria, 301 (2011) 1-12)

**CERE 1006** "Evaluation of the CO<sub>2</sub> Behavior in Binary Mixtures with Alkanes, Alcohols, Acids and Esters Using the Cubic-Plus-Association Equation of State" • Mariana B. Oliveira, António José Queimada, Isabel M. Marrucho, Georgios M. Kontogeorgis, and Ioão A.P. Coutinho

(Journal of Supercritical Fluids, 55 (2011) 876-892)

CERE 1007 "Upscaling of Two-Phase Immiscible Flows in Communicating Stratified Reservoirs" • Xuan Zhang, Alexander Shapiro, and Erling H. Stenby (Transport in Porous Media, 87 (2011) 739-764

CERE 1015 "Towards Predictive Association Theories"

- DOI: 10.1007/s11242-011-9713-1)

• Georgios M. Kontogeorgis, Ioannis Tsivintzelis, Michael L. Michelsen, and Erling H. Stenby (Fluid Phase Equilibria, 301 (2011) 244-256)

**CERE 1018** "Analysis and Application of GCPlus Models for Property Prediction of Organic Chemical Systems"

 Azizul Azri Mustaffa, Georgios M. Kontogeorgis, and Rafigul Gani

(Fluid Phase Equilibria, 302 (2011) 274-283)

**CERE 1021** "An Explanation of the Selective Plating of Laser Machined Surfaces using Surface Tension Components"

• Yang Zhang, Georgios M. Kontogeorgis, and Hans Nørgaard Hansen

(Journal of Adhension Science and Technology, 25 (2011) 2101-2111)

**CERE 1023** "Experimental Determination and Modeling of the Phase Behavior for the Selective Oxidation of Benzyl Alcohol in Supercritical CO2" Ioannis Tsivintzelis, Matthias Josef Beier, Jan-Dierk Grunwaldt, Alfons Baiker, and Georgios M. Kontogeorgis

(Fluid Phase Equilibria, 302 (2011) 83-92)

CERE 1024 "Mutual Solubility of MEG, Water and Reservoir Fluid: Experimental Measurements and Modeling Using the CPA Equation of State"

and Ioannis G. Economou

CERE 1027 "Application of Association Models to Mixtures Containing Alkanolamines" Ane S. Avlund, Daniel K. Eriksen, Georgios M. Kontogeorgis, and Michael L. Michelsen (Fluid Phase Equilibria, 306(1) (2011)31-37)

Equation of State"

Filtration Systems"

**CERE 1041** "Uncertainty and Sensitivity Analysis of Filtration Models for Non-Fickian Transport and Hyperexponential Deposition" • Yuan Hao, Gürkan Sin (Chemical Engineering Journal, 168(2) (2011) 635-648)

CERE 1047 "Measurement and Modeling of CO<sub>2</sub> Solubility in NaC1 Brine and CO<sub>2</sub>-Saturated NaC1 Brine Density" • W. Yan, S.L. Huang, and E.H. Stenby (International Journal of Greenhouse Gas Control, 5 (2011) 1460-1477)

Muhammad Riaz, Georgios M. Kontogeorgis, Erling H. Stenby, Wei Yan, Toril Haugum, Kjersti O. Christensen, Even Solbraa, and Torbjørn V. Løkken (Fluid Phase Equilibria, 300 (2011) 172-181)

**CERE 1025** "Partition Coefficients of Organic Molecules in Squalane and Water/Ethanol Mixtures by Molecular Dynamics Simulations" Rasmus Lundsgaard, Georgios M. Kontogeorgis,

## (Fluid Phase Equilibria, 306(2) (2011) 162-170))

CERE 1028 "Modelling of the Thermodynamics of the Acetic Acid-Water Mixture using the CPA

• Martin P. Breil, Georgios M. Kontogeorgis, Paul K. Behrens, and Michael L. Michelsen

## (Industrial & Engineering Chemistry Research, 50(9) (2011) 5795-5805)

CERE 1031 "Modeling Phase Equilibria for Acid Gas Mixtures using the CPA Equation of State. Part II. Binary Mixtures with CO2"

 Ioannis Tsivintzelis, Georgios M. Kontogeorgis, Michael L. Michelsen, and Erling H. Stenby (Fluid Phase Equilibria, 306 (2011) 38-56)

CERE 1039 "A Mathematical Model for Nonmonotonic Deposition Profiles in Deep Bed

• Hao Yuan, and Alexander Shapiro

(Chemical Engineering Journal, 166 (2011) 105-115 - DOI: 10.1016/j.cej.2010.10.036)

## New manuscripts in 2011 **CERE 1101** "Properties of Cryobrines on Mars" Reservoirs" • D. Möhlmann, and K. Thomsen (Icarus, 212 (2011) 123-130) CERE 1102 "Novel Self-Associative and Multiphase Nanostructured Soft Carriers based on Amphiphilic Hyaluronic Acid Derivatives" Pressure Data" Corinne Eenschooten, Andrea Vaccoro, • I.L. Fabricius, and M.A. Rana Florence Delie, Fanny Guillaumie, Kristoffer Tømmeraas, Georgios M. Kontogeorgis, Khadija Schwach-Abdellaoui, Michal Borkovec, and (2011) 463-472) Robert Gurny (Carbohydrate Polymers, 87(1) (2011) 444-451) **CERE 1103** "High-Pressure Fluid-Phase Fabricius Equilibria: Experimental Methods and Systems Investigated (2005-2008) • José M.S. Fonseca, Ralf Dohrn, and Stephanie Peper (Fluid Phase Equilibria, 300 (2011) 1-69) Temperatures" CERE 1104 "Intramolecular Association within the SAFT Framework" Foged • Ane S. Avlund, Georgios M. Kontogeorgis, and Walter G. Chapman (Molecular Physics, 109(12) (2011) 1759-1769) CERE 1105 "Competitive Adsorption of Nitrogen Compounds in the Hydrodesulfurization of 4.6-Dimethyldibenzothiophene" • Rasmus R. Boesen, Nicolas S. von Solms, greensand" Michael L. Michelsen, Rasmus G. Egebjerg, and Kim G. Knudsen (Submitted to Chem. Eng. Sci) CERE 1106 "Measurement of Liquid-Liquid Equilibria for Condensate + Glycol and Condenporous media" sate + Glycol + Water Systems • Muhammad Riaz, Georgios Kontogeorgis, Erling H. Stenby, Wei Yan, Toril Haugum, Kjersti

Christensen, Torbiørn Løkken, Evan Solbraa (Journal of Chemical & Engineering Data, Kenneth N. Marsh Festschrift, doi:10.1021/ je200158c)

**CERE 1107** "Freezing Point Depressions of Aqueous MEA, MDEA, and MEA - MDEA Measured with a New Apparatus" • Philip Loldrup Fosbøl, Mikkel Gielsager Pedersen, and Kaj Thomsen (Journal of Chemical Engineering Data, 56 (2011) 995-1000)

**CERE 1108** "Induced Migration of Fines during Waterflooding in Communicating Layer-cake

 Hao Yuan and Alexander Shapiro (Journal of Petroleum Science and Engineering, 78 (2011) 618-626)

**CERE 1109** "Tilting Oil-Water contact in the Chalk of Tyra Field as interpreted from Capillary

(Petroleum Geology Conference series, 7

CERE 1110 "Petrophysical Properties of Greensand as Predicted from NMR Measurements" • Z. Hossain, C.A. Grattoni, M. Solymar, and I.L.

(Petroleum Geoscience, 17 (2011) 111-125)

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