DTU

Annual Report 2012

# CERE

Center for Energy Resources Engineering

Technical University of Denmark

## CERE Annual Report 2012

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The photo shows tailor-made end caps from high pressure cylinders.
Photo: Christian Ove Carlsson, CERE DTU

# Contents

# Dear Partners, Members and Colleagues!

Erling H. Stenby
Chairman of CERE,
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CERE's ability to attract the sharpest young minds and talents from around the world plays a key role in our success and growth as a research center

2012 was a good year for CERE. The research programs initiated during the last two years left the initial phases and began to produce new and valuable results. At the same time, our consistent funding and innovation efforts paid off as we attracted yet another large interdisciplinary research project looking into challenges related to High Pressure - High Temperature oil and gas production. A string of smaller projects and spin off activities found proper funding as well, and I'm confident to say that we enter 2013 with great optimism regarding the future research and cooperation opportunities.

It was a good year in many ways, but when I look back at the past 12 months, it is neither the research nor the funding that strikes me as the biggest achievement: it is our ability to attract talents and the growing name CERE has among young talents from very different scientific communities around the world.

## Proud of our PhD's

CERE is an independent, university based, research unit. The education and training of MSc and doctoral students are some of the most important aspects of our activities, and many of our member companies invest a lot of effort in supporting them in the pursuit of a highly trained, professional work force. We are proud of our PhDs, and we are happy to see, that they all successfully continue their careers in attractive positions where their undisputable talent and learned skills as researchers are put to good use.

Talent is the key word here, for it is undoubtedly CERE's ability to attract the sharpest minds and talents that plays the key role in our consistent success. Of course we train people well and of course CERE senior staff constitutes a highly skilled group of mentors. But at the end of the day, it is the combination of quality and sheer numbers of talented young people we attract that impresses me and our end users. I consider this a major achievement at a time when many science departments struggle to recruit the right people, and I promise that this will be a major focus area for CERE in the years to come.

## A unique blend

Besides CERE having made a name for ourselves, I believe that our power to attract talent is supported by the unique blend of disciplines in our research organization. Thanks to our expertise in selected areas and the vision for strong interdisciplinary collaboration, we can handle a wide array of problems and produce new insights and robust solutions to crucial energy related questions where others have to give up.

CERE is growing, but it is an organic, robust growth governed by the needs of our end users and the availability of the right talent and the right competences. We are not pursuing a large, department-like structure. We will continue to be a relatively small, agile taskforce of competent senior scientists working with the best talents from around the world taking on specific challenges and problems facing our member companies and society.

*Professor Erling H. Stenby,*
*Chairman of CERE*

*A more detailed summary of 2012 events to be found on page 25.*

# The Consortium – our Strongest Asset

CERE is supported by public means from several sources, e.g. The Danish Research Council for Technology and Production Sciences and Danish National Advanced Technology Foundation. Furthermore, the Center is supported by grants from several private companies. The strongest asset of CERE is the industrial Consortium. 28 companies are members; the exact number changes due to the dynamics of the industry's mergers and acquisitions. The member companies follow the activities of the Center closely. This ensures that CERE activities are relevant in relation to the topical problems and limitations of existing knowledge within applied thermodynamics. This ongoing external control of quality and inspiration maintain CERE research at the highest international level.

## We welcome Hess

Hess Corporation is a leading global independent energy company engaged in the exploration and production of crude oil and natural gas, as well as in refining and in marketing refined petroleum products, natural gas, and electricity. In 2011, crude oil and natural gas production was 370,000 barrels of oil equivalent per day. Proved reserves stood at 1.573 billion barrels of oil equivalent, and the company's reserve life was 11.4 years. Hess Corporation has been active in the Danish part of the North Sea for a number of years.

## We welcome Infochem

Infochem is a leading supplier of thermodynamic software and consultancy services to the oil and gas industries. By June 2012 Infochem was acquired by KBC. With over 30 years of experience and operating out of 14 global locations, KBC provides independent consultancy to the global energy and process industries, combining advanced software with experienced engineers and operations personnel. The acquisition expanded KBC interest in upstream energy industry, as Infochem brought software and intellectual property rights within the chemistry of oil and gas fluids that enable flow assurance and other types of modeling of reservoir fluids to maximize production.

PHOTO: HESS

PHOTO: KBC

### CERE Consortium:

- Akzo Nobel
- BP
- Chevron
- ConocoPhillips
- DONG Energy
- Eni
- ExxonMobil
- GASSCO
- GDF-SUEZ
- Haldor Topsøe
- Hess
- IFP
- InfoChem
- Linde
- Lloyd´s Register ODS
- Maersk Oil
- National Oilwell Varco
- OMV
- Petrobras
- RWE
- Schlumberger
- Sinopec
- Shell
- Statoil
- SQM
- Total
- Vattenfall
- Welltec

# Deep Reservoirs are within Reach

Significant reserves of oil and gas are present in reservoirs at larger depth than those presently being produced in the North Sea. A new scientific program led by CERE addresses the task.

It was a major surprise in itself when oil was first found in the chalk layers below the seabed of the North Sea back in the 1960's, and now a further text book revision is due. Earlier it was considered that high temperature and pressure at depths of several kilometers would exclude the presence of oil and gas. In recent years investigations have revealed that oil and gas are indeed present.

Recently, DONG Energy has decided to produce the Hejre field located at 5000 meters depth. The company is a partner to the NextOil DK research program initiated November 1st 2012. The other partners are Maersk Oil, GEO, and CERE.

"The program will support the efforts of DONG Energy in producing the Hejre field. Further, we hope that the results will play a part in the foundation for strategic decisions regarding exploration at even larger depths," says Professor Erling Stenby, CERE Chairman and Chairman of the scientific advisory board of NextOil Dk.

## High Pressure, High Temperature

As depth increases, so does both temperature and pressure. The temperature increase is caused by the greater proximity to the Earth's hot core, while the high pressure is due to the weight of the overlying layers. Thus oil exploration at large depth is known as HPHT: High Pressure, High Temperature. The pressure at the Hejre field is 1000 bars, while the temperature is 160 degrees °C. According to DONG Energy, the fields' exploitable oil and gas reserves amount to 171 million barrels of oil equivalents. Production is scheduled to commence by the end of 2015.

"The global oil and gas community needs a stronger knowledge base to handle the challenges of High Pressure High Temperature production . In the new NextOil project, we aim to establish a strong research task force and facility capable of delivering some of the much needed answers and solutions for the future HPHT production. We expect the facility to become a key player at HPHT-related research, not just in Denmark but also internationally," Chairman Erling Stenby states.

## Focusing on environment and security

NextOil DK is organized as three work packages. Rock mechanics is the headline of work package I, which is led by professor Ida L. Fabricius, CERE.

*The pressure is on. Data from relevant experiments conducted under the high pressure present under oil and gas production at large depth are scarce in the scientific literature. Financing from the NextOil DK program has allowed CERE to establish a strong facility dedicated to the purpose.*


PHOTO: DONG

"We are already considering how we should make the most of the Danish North Sea resources. However, we are aware that as we move to a certain depth and at special conditions, a number of variables are still unknown. We need to grasp all opportunities for gaining further knowledge of these unknown variables in order to be able to produce even more oil and gas in a secure and responsible way in the future. Our latest North Sea investment, the Hejre field, is HPHT and shows that we in Denmark too can gain from a better understanding of oil production in deep fields. Hopefully, this research will also come into play in other parts of the world."

Søren Gath Hansen, Executive Vice President, responsible for Exploration and Production, DONG Energy.

"It is a key question how the geological structure will be affected as production begins. It would be highly unfortunate if the structure around a production well were to collapse. Given that the cost of setting up an HPHT well is considerably higher then other offshore installations, a huge investment would be lost if the well were to cease production after, say, just a few months," Erling Stenby explains, adding that environmental and safety concerns are also a focuspoint of NextOil DK:

"In a worst case scenario, oil and gas could leak or even blow-out. We are very aware of the safety issues, and as always, we are even more cautious when commencing a new type of activity."

## High concentrations of salts

Besides having overall responsibility for the NextOil DK program, senior scientist Wei Yan, CERE, heads work package II, which is dedicated to reservoir fluids. The package comprises both a large experimental side to provide extensive new data under realistic HPHT conditions and a large modeling side which will aim at adjusting present thermodynamic models and simulation tools in order to assure that they remain reliable under HPHT conditions.

Finally, work package III, led by associate professor Kaj Thomsen, CERE, relates to scaling, which is precipitation of inorganic salts from water present in the reservoirs. It is known from other types of oil and gas exploration that the precipitation of salts in the well and the surrounding rock will increase as production is initiated. It is not possible to apply this type of experience directly from other types of production to HPHT, Erling Stenby stresses:

"Firstly, we know that concentrations of dissolved salts can be very high in HPHT-reservoirs. Secondly, we know that a number of the tools normally available to control and chemically adjust precipitation of salts during production are just not applicable under HPHT conditions. And finally, it could well be that different salts will be precipitated at HPHT – we are not sure of this, but we will look into it. All in all this is a field one needs to give attention."

## Enhanced Oil Recovery ideas

Most fields currently in production in the Danish part of the North Sea are carbonate which is challenging in terms of oil recovery. The HPHT fields are found in quite different geological structures, including sandstone, which generally provides better conditions for recovery.

"Therefore the question of recovery rate is not quite as urgent in this context as regarding the carbonate reservoirs. One should also remember that these are additional reserves, meaning that regardless of the final recovery rate obtained, the fields will add to the total expected production in the Danish part of the North Sea," Erling Stenby says, while noting:

"Nevertheless it is a part of our nature to consider if the experience around enhanced oil recovery in carbonate reservoirs can be applied in optimizing HPHT recovery. Unfortunately, water flooding is technically impossible to apply under these conditions. We have some alternative ideas, but it would be premature to elaborate on them."

## NextOil DK

The NextOil DK program is focused at HPHT (High Pressure High Temperature) oil and gas exploration in the Danish part of the North Sea. Partners are DONG Energy, Maersk Oil, GEO, and CERE heading the program. The program has a budget of 4.6 million EUR, of which 2.0 million EUR are provided by The Danish National Advanced Technology Foundation (Højteknologifonden), and the rest by the partners. The program began November 1st, 2012 and is scheduled to run for four years.

"The North Sea is still rich in resources. The time has come to address oil and gas reservoirs that are less easy to produce from. The NextOil DK project will be able to provide a significant contribution to the safety of the environment, to the safety of our employees involved in production, and to the society as a whole in order to ensure that the remaining amounts of oil can be produced in a safe and effective manner."
**Morten Stage, lead geomechanical specialist, Maersk Oil.**

# A firmer Grip of Complex Mixtures

2012 saw several breakthroughs in modeling of multicomponent multiphase equilibria of mixtures containing hydrocarbons, gases, water, and other polar chemicals. Also, unique experimental data was obtained.

Consistent efforts by CERE and a number of its industry Consortium participants to develop better tools for modeling of contemporary oil and gas production was rewarded by significant progress in 2012. Joined in the Chemicals in Gas Processing (CHIGP) project headed by Professor Georgios Kontogeorgis, the partners have for 10 consecutive years developed models which are useful for thermodynamic calculations for mixtures of relevance to the petroleum and chemical industries.

Modern recovery often results in mixtures of oil and gas with hydrate inhibitors – methanol and glycols – and organic acids. Such polar and hydrogen bonding compounds are difficult to handle with conventional models used in oil industry like cubic equations of state. Instead a rigorous thermodynamic model, the CPA (Cubic-Plus-Association) equation of state has been developed in the CHIGP project.

## CHIGP

2012 was the 10th consecutive year of the joint industrial project of CERE, called CHIGP (Chemicals for Gas Processing). Current participants are Statoil (Norway), GASSCO (Norway), BP (UK), DONG Energy (Denmark), and Petrobras (Brazil). Previously (in the periods 2004-2009 and 2006-2011), TOTAL (France) and Maersk Oil (Denmark) have also participated.

All results are immediately disseminated to the participating companies via CERE's web-site and especially via a special project web-site on www.chigp.dk.

The deliverables include software in the form of CAPE-OPEN compliant modules and user-models for the ASPEN process simulator. In this way, the results can be used by industry almost as soon as they are produced. PhD student Bjørn Maribo-Mogensen is the software manager of the center and is also in charge of the computational developments in CHIGP.

Moreover, the results are presented in progress meetings held twice a year; 18 meetings have been held since 2003, and the next is planned for May 2013.

In addition to extending the CPA model to new mixtures of industrial and scientific significance, robust algorithms for complex thermodynamic calculations and parameter estimation are being developed and new experimental measurements carried out when necessary in order to support the model development. Such measurements are often being carried out in collaboration with industrial partners of the CHIGP consortium.

### Unique experimental results

In the period 2010-2012, a series of experimental measurements was performed at the research center of Statoil (Norway). In the experiments, five different oils have been considered so far. These measurements are unique in the sense that only very few similar data on oils with polar chemicals are available in the literature. These data permitted the validation of CPA for "real oil" mixtures with very promising results. It is clear that CPA offers a successful alternative to cubic equations of state and is a good compromise between accuracy and simplicity.

The experiments at Statoil were undertaken by CERE PhD students Muhammad Riaz (PhD, 2011) and Michael Frost and M.Sc. student Mustaffe Jussuf. Muhammad Riaz's and Michael Frost's projects are the most recent in a long list of PhDs funded by Statoil within the CHIGP framework.

In addition, Michael Frost has worked closely with professor Dominique Richon (who visited CERE during the summer 2012) optimizing existing equipment for vapor-liquid measurements and designing a novel apparatus which will be able to perform multiphase (vapor-liquid-liquid equilibrium) measurements over extensive temperature/pressure ranges.

### Collaboration on sulfur compounds

The CPA work during 2012 has focused on four directions: oil-related systems, acid gas mixtures (especially with $CO_2$), electrolytes, and chemicals.

The work on oil-related systems has followed two complementary directions: Well defined chemicals relevant to petroleum applications and reservoir mixtures. In the well-defined chemicals work, the efforts of CHIGP have focused on the important gas hydrate inhibitors (methanol, glycols) and on mercaptanes and other sulfur compounds.

The mercaptanes study has been carried out in the framework of the two-year post-doctoral grant (2011-2012)

PHOTO: ØYVIND HAGEN/STATOIL

awarded to Dr. Javeed Awan from the Danish Research Council. In this project, measurements and modeling for mixtures containing mercaptans, such as sulfur compounds of importance to oil industry, have been carried out. These measurements are quite difficult and require special equipment and safety regulations. They have been carried out by Javeed Awan at Ecole de Mines in France. All systems subsequently have been modeled successfully with CPA.

### An improved CPA for $CO_2$ hydrates

Acid gas is another major subject of interest in CHIGP. The work of Dr. Ioannis Tsivintzelis has established that CPA can predict multicomponent multiphase equilibria of mixtures containing acid gases ($CO_2$, $H_2S$), hydrocarbons, water, and other polar chemicals (alcohols, glycols) over extensive temperature and pressure ranges.

Overall the best results are obtained when solvation is accounted for between the acid gases and the polar chemicals. This stage of the project is completed, however the acid gas work will be continued during 2012-2014 due to the research grant "$CO_2$ Hydrates – Challenges and Possibilities" which has been obtained from the Danish Technical Research Council.

The project is in collaboration with Ecole des Mines (Dr. Amir Mohammadi and Dr. Christophe Coquelet) and has a budget of about 640,000 Euro. It involves two sub-projects: Modeling of $CO_2$ hydrates using "an improved CPA" which includes a quadrupolar term, and experiments for $CO_2$ hydrates with promoter. PhD student Martin Gamel Bjørner is employed in sub-project 1, while sub-project 2 will start in 2013.

### New results for biodiesel

2012 marked significant developments in the development of an electrolyte CPA carried out in Bjørn Maribo-Mogensen's PhD project (2011-2014). The project aims to develop a model that can predict gas solubilities in mixed solvents containing salt and calculate conditions for gas hydrate formation.

Results have shown that major theories for accounting for electrostatic interactions (MSA vs. Debye-Hückel) perform very similarly unlike what was previously thought. Further, Bjørn Maribo-Mogensen has developed a predictive model for the static permittivity of solvent mixtures with electrolytes. Finally, the first results with the e-CPA description of osmotic coefficients for aqueous salt solutions are very promising.

During 2012, CPA has been applied to different complex chemicals: Ionic liquids (with guest PhD student Filipa Maia from the group of professor E. Macedo in Portugal), multicomponent mixtures with acetic acid, alcohols, ethers, and esters, and especially the extensive work carried out by Dr. Tsivintzelis on modeling chemicals and mixtures related to biodiesel (glycerol, heavy esters, etc.). Modeling of acetic acid mixtures remains a significant challenge, while the results for biodiesel related mixtures are very satisfactory considering the uncertainties in the experimental data.

*Modern oil recovery often includes complex mixtures, not least under cold conditions where hydrate inhibitors need to be present in significant quantities. In the CHIGP project, a thermodynamic model the Cubic Plus Association equation of state is maintained as an extension of traditional models used in the oil and gas industry.*

Experiments performed at the research center of Statoil have established that CPA offers a good compromise between accuracy and simplicity.

*Over the past ten years, the market value of Petrobras has increased seven times. The Brazilian company is looking to expand its deep water activities further over the coming years.*

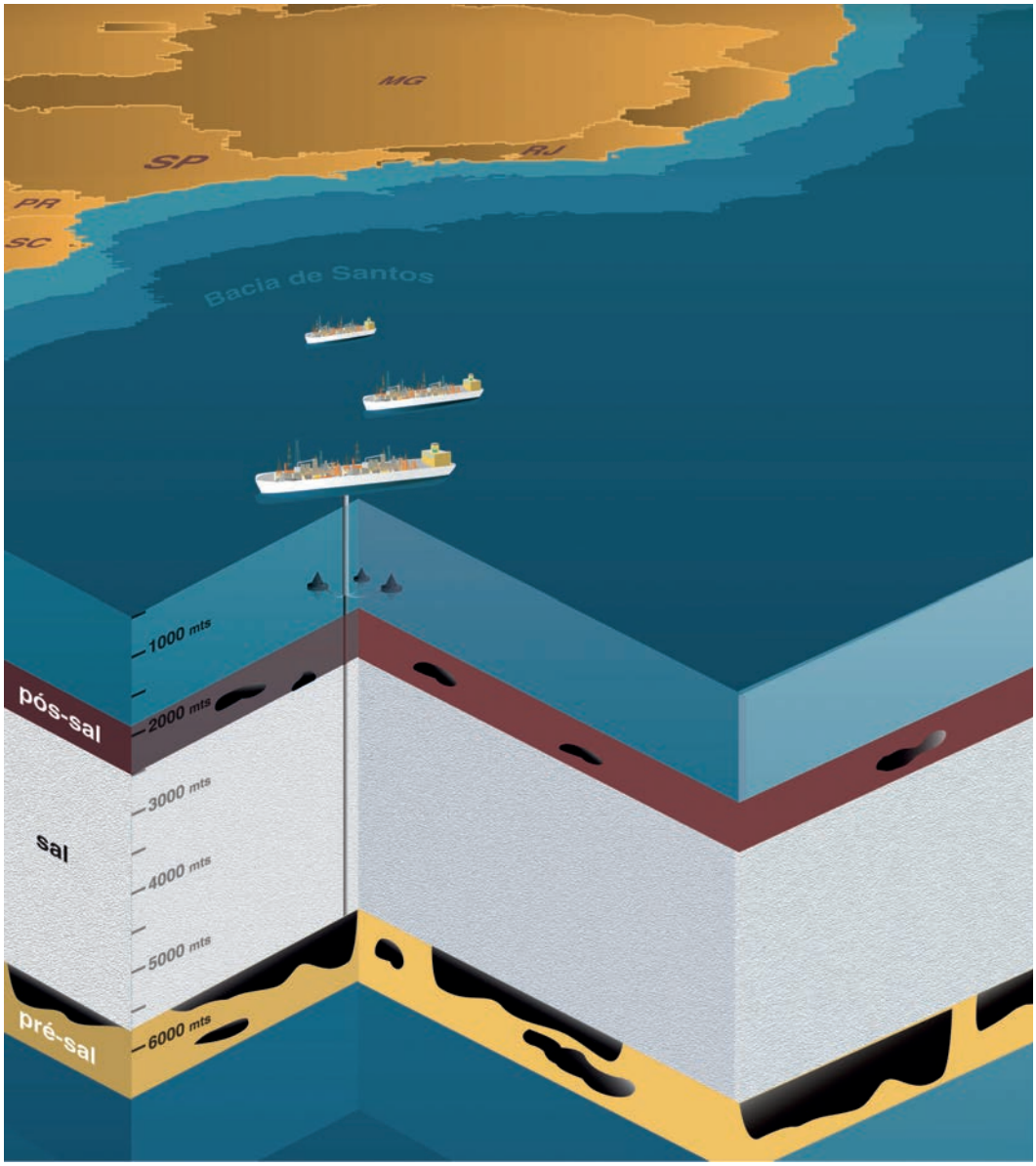



ILLUSTRATION: PETROBRAS

# Petrobras joins CHIGP

The most recent CHIGP participant is Petrobras. The Brazilian energy company is active in oil and gas exploration and processing, petrochemicals and fertilizers, as well as in bio fuels production. Over the past ten years, the market value of Petrobras has increased seven times. The company produces 2.6 million barrels of oil and more than 43,000 cubic meters of gas per day, representing more than Brazil's total demand.

"Petrobras is very committed to research and development. The R & D investments are not confined to only internal or just Brazilian institutions, but include foreign universities and joint research projects. The CERE Consortium and the CHIGP project is part of that policy," says Dr. Leticia Cotia dos Santos of Petrobras Downstream Gas and Power R & D.

Most of the oil refined by Petrobras is domestic, and the company is engaged in developing novel refining technologies and process schemes.

"Moreover, as the deep water oil and gas production has increased, there are more issues to answer and more challenges. As the process designs are elaborated with a high degree of innovation, the utilization of an in-house process simulator has strategic advantages," Leticia Cotia dos Santos explains, adding:

"In this scenario, building process models and implementing these in simulators are very important parts in the technology development. PETROX, Petrobras' process simulator, is a fruit of this conception. This is where the CPA equation of state, developed in CHIGP, will be applied."

# Microbes and Enzymes for Oil Recovery

Identification of a potent enzyme and confirmation of bacteria being able to penetrate tight chalk are two notable milestones in the first year of a CERE-led program on biotechnology in oil recovery.

Everybody wants something green and cheap...

In just six words PhD students Alsu Khusainova and Amalia Yunita Halim sum up the main challenge facing the Biotechnology in Oil Recovery (BioRec) program. In a joint effort with two Danish energy corporations, Maersk Oil and DONG Energy, and the world's leading enzyme producer, Novozymes, CERE embarked on an ambitious quest last year. The BioRec program aims to create the scientific foundation for introducing microbial and enzymatic enhanced oil recovery (EEOR) methods in full-scale recovery.

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

With significant funding from the partners and from the Danish Advanced Technology Foundation, the BioRec program is at the cutting edge of this development.

## Adding microbes to tight chalk

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 adding microbes to a field in order to increase production is less than four years old. This concept, involving exogenic bacteria, is part of Amalia Yunita Halim's PhD project which was initiated in February 2012 under BioRec. She outlines the first challenge which had to be overcome:

"As the BioRec program is focused at the Danish part of the North Sea, characterized by tight carbonate reservoirs, it was by no means a given thing that it would even be possible to introduce exogenic bacteria to a reservoir."

## Bacteria can adjust their shape

Several of the bacteria of interest have sizes in the same range as the pores of the chalk.

"Of course it would be pointless to focus at a certain bacteria, if it is simply not applicable," Amalia Yunita Halim says, adding:

"Fortunately, our experiments have shown that it is indeed possible to introduce the bacteria. The microbes are flexible to a point where they can even adjust the shape of the individual cells, allowing them to penetrate at critical pore sizes."

On these grounds, Amalia Yunita Halim and her co-workers can now continue their investigations, focusing mainly on two groups of exogenic bacteria: the Bacillus licheniformis (spore forming) and the Pseudomonas putida (non-spore forming). In the coming phase, oil/brine interactions will be in focus.

Besides plainly evaluating the capability of these microbes in increasing oil recovery, the science aims at understanding the mechanisms involved. One suggestion is that bacteria work by reducing the interfacial tension (IFT) due to surfactant production. However, several alternative explanations can be imagined. Understanding of the mechanisms is likely to be crucial to suggesting the right bacteria and method of application for a given purpose.

## Starting from scratch on enzymes

With regard to enzymes, it is known that certain enzymes can enhance oil production in chalk in much lower concentrations compared to chemical surfactants. The first step in the BioRec project is to check whether enzymes 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, making it more water-wet. This is what enzymes do, for example, in washing powder.

Enzymes are the subject of Alsu Khusainova's PhD project, initiated in December 2011 and conducted in close cooperation with Novozymes:

"To start with we had even less information on enzymes compared to microbes. We practically had to start from

> The microbes are flexible to a point where they can even adjust the shape of the individual cells to penetrate at critical pore sizes.
> **Amalia Yunita Halim, PhD student, BioRec**

zero. Fortunately, the technical personnel here at CERE are highly experienced. They have helped me a lot in setting up the experiments, giving advice that you cannot see in any text book."

### Enzyme candidate at hand

From a range of candidates proposed by Novozymes, the project has identified one type as particularly interesting for the purpose. The enzyme group in question is the socalled lipases well known from several other contexts, i.e. they are widely used in the food industry and in detergents. Based on a range of criteria including wettability alteration, ability to influence contact angle favourably and adhesion behaviour, certain lipases have been picked for further study.

"We will not claim that these species are optimal for full scale recovery, even though they are promising in the lab. Given the high temperature and pressure and other special conditions in a real reservoir, it would in fact be unlikely that the same enzymes should function," Alsu Khusainova explains.

"However, we can utilize our studies to identify the critical features an enzyme should have for the purpose. We can then ask Novozymes to manufacture a novel enzyme with the same features, but resistant to reservoir conditions. The company has a long track record of producing optimal enzymes for specific purposes."

### Staying calm under time pressure

At the 2012 version of CERE's Discussion Meeting, several industry participants focused on the need to develop EOR methods for the North Sea quickly, as many installations are to be decommissioned in a not too distant future. Challenged with the notion of time pressure, Alsu Khusainova calmly replies:

"Well, we are already in a time squeeze, as we only have three years to finish our PhD projects. I am sure all PhDs want to obtain results within this relatively short time frame. Also, this is experimental work. Many things can go wrong – and some of them will go wrong. You cannot force these things forwards. If you try, you will just encounter more problems."

Amalia Yunita Halim joins in:

"Yes, we feel the pressure in any case. Besides our research we need to follow a number of courses and fulfill other obligations."

However, both PhD students have noticed the eagerness of the industry participants:

"We have work package meetings every three months. These are very fruitful. We get a lot of inspiration from the industry participants. Also these sessions function as deadlines for us. We are very aware that we are expected to report some kind of progress each time", says Alsu Khusainova.

### Results won't be left on the shelf

Alsu Khusainova goes on to underline that she is keen to see results applied:

"Actually, the close cooperation with the industry was one of the main reasons why I applied for the position. I feel confident that results will not be left on the shelf."

However, the time frame for application does not just depend on the efforts of the researchers, she stresses:

"A lot of infrastructure and logistics need to be developed in order to put microbial and enzymatic enhanced oil recovery into full scale practise. Just to take an example, the use of microbes or enzymes will probably rely on development of special tanks for the purpose."

"In many contexts, it is quite normal that it takes about ten years from a scientific breakthrough until the result is seen in a commercial application. An attractive feature of the oil industry is that it is very dynamic. If we obtain really convincing results, I think that it would be realistic to see them put into practise in just, say, five years."

> The close cooperation with the industry was one of the main reasons why I applied for the position (...) results will not be left on the shelf.
> **Alsu Khusainova, PhD student, BioRec**

*Scientists and industry participants in BioRec meet frequently to evaluate progress. Seen at the project's first annual event in January 2012 are PhD students Amalia Yunita Halim, Christine Malmos and Alsu Khusainova*

# Energy Scientists in a Time Squeeze

The annual Discussion Meeting is where the members of CERE's industrial Consortium and the researchers mingle in order to exchange ideas. Reaching across disciplines as always, the 2012 version was the largest and most diverse meeting in the 30 years history of CERE.

"The researchers will need to pull up their sleeves. New methods for increasing the rate of oil exploration in the Danish part of the North Sea may not have an impact if they are not in place within the next five or ten years, since we will begin decommissioning our offshore installations in the near future in case we cannot change the current downward trend in production rates. We are really in a time squeeze here."

Dr. Finn Engstrøm of Maersk Oil was frank as he addressed the 2012 version of CERE's Discussion Meeting, and judging from the intense buzzing during coffee breaks later that day, his message came through loud and clear.

The annual conference is a tradition which has just grown stronger over the years. With 34 industry participants representing 17 companies from 10 countries, the 2012 version held at the Pharmakon conference centre in Hillerød once more demonstrated CERE's position as one of the most influential research groups in this field.

"Every year, we are honoured to see that representatives from our industrial Consortium find it important to sit down with our Faculty and discuss future challenges and important tasks for CERE ," CERE Chairman, Professor Erling Stenby, noted.

### A huge EOR potential

The list of participants showed representation from a wide range of industries. In his presentation, Dr. Finn Engstrøm, Maersk Oil, summed up the situation for oil exploration in the Danish part of the North Sea:

"We have produced about 25 per cent of the discovered volumes of oil in chalk reservoirs and expect to produce another 10 per cent. Originally, it was feared that only 2-3 per cent could be extracted, but progress in methods like horizontal wells, water injection, and recently the application of the FAST (Fractured Aligned Sweep Technology) water flooding technique has improved the situation by a

"What I like about this conference is that people are not afraid of putting a bunch of equations up there.
**Dr. Graeme Keith, DONG Energy**

"Just like you have experienced in the Danish part of the North Sea, we see challenges in developing carbonate reservoirs in China.
**Dr. Zengmin Lun, Sinopec**

"The Discussion Meeting is a nice opportunity to get a picture of who are able to solve the kind of problems that are relevant to our business.
**Dr. Jim Bennett, Schlumberger**

*In his presentation, Dr. Finn Engstrøm, Maersk Oil, stressed the urgency in improving recovery rates in the North Sea.*

factor of 10-20. But of course there is a large scope left for further improvements," Finn Engstrøm said, illustrating:

"Just to give an example, we know that oil equivalent to the total consumption in Denmark during 10 to 15 years is left at the chalk reservoirs if we leave just a 5 nanometer thick layer of oil on the chalk surfaces."

More specifically, Finn Engstrøm called for further progress within reservoir simulations, history matching, basic chalk geology, and also regarding several novel Enhanced Oil Recovery (EOR) methods.

## Calling for a government policy

Finn Engstrøm went on to state that not only scientists are in a time squeeze:

"Companies need to improve their ability to absorb new knowledge faster. And governments needs to understand the value of continuous oil production for our society."

Various presentations during the meeting showed how the joint efforts of CERE's researchers and the Consortium members have already produced progress in a range of fields relevant to EOR and discovery of new oil and gas resources.

*The annual Discussion Meeting is a tradition which has just grown stronger over the years.*

Especially a presentation by PhD. student Andrea Capolei, DTU Compute, brought pleased smiles to the faces of several industry participants. A new approach developed by the geophysics group at CERE promises to improve the value-cost ratio of water flooding in uncertain geological conditions significantly.

Other new findings with direct applications in oil and gas discovery and enhanced recovery were also presented; e.g. in history matching, chalk geology, gas hydrate inhibition, enzymatic and microbial enhanced oil recovery, and thermodynamic modeling of complex mixtures.

## An inspirational format

Dr. Raghuraman Pitchumani, Senior Research Thermodynamicist at Shell Global Solutions International, Netherlands, is a first-time Discussion Meeting participant. He finds the format interesting:

"While normally, conferences are shattered in too many parallel sessions, here speakers present the same content to all participants. This gives a pleasant atmosphere. Of course the downside is that you sometimes spend time listening to presentations on topics that are not relevant to your daily work. But I have found that this can be surprisingly inspirational. Earlier today for instance, I was listening to a presentation on processing of seismic data. As I work in thermodynamics, seismic data are not a part of my work, but the presentation actually brought some ideas to my mind. I will take them into discussions with other groups at Shell."

Another attractive feature of the meeting is the length of the presentations, which are generally held at 20 minutes each.

"Not too long, not too short," Raghuraman Pitchumani states, adding:

"My observation is that we have not had the speakers facing too many questions from the audience – but here I am also guilty! On the other hand you have many occasions to catch up during intervals and poster sessions asking your questions personally. In this way I feel that I have had discussions with CERE's experts and other participants on the topics I am interested in."

## Strong presence from Sinopec

China Petroleum & Chemical Corporation – or Sinopec Corp - joined the CERE industrial Consortium in 2009. The company, today one of the world's largest energy corporations, maintained a strong presence at the 2012 event with six representatives. The delegation was headed by Dr. Zengmin Lun who was attending for his third time.

"As an international company, Sinopec is keen to cooperate with leading research groups abroad. We have already collaborated with the DTU for some years now and as we have learned how to run our cooperation in a fruitful way in relation to the advanced technology involved and

other forms of mutual support, we are happy with the cooperation and expect to expand it further," says Dr. Lun.

Among the topics of high interest to Sinopec at the 2012 meeting is Enhanced Oil Recovery.

"Just like you have experienced in the Danish part of the North Sea, we see challenges in developing carbonate reservoirs in China. These reservoirs are more complex than sandstone reservoirs, and it is natural that experts in these reservoirs cooperate internationally," Zengmin Lun states.

### "In the beginning was the cubic"

As always, a lengthy session at the event was dedicated to thermodynamic modeling. Especially professor Michael Michelsen had the audience's full attention as he summed up experience gained over the past decade within calculation of phase equilibrium.

"In the beginning was the cubic," Michelsen said, going on to quote Dr. Jack Heidman of ExxonMobil, who attended a similar meeting at DTU in the late 1990's:

"Cubic equations of state are here to stay, Dr. Heidman said, but while I admit, that yes, they are still here, my feeling is that they will not be here forever."

Cubic equations are known to be the simulation work horses of the oil industry. CERE has been heavily involved in an improved tool, the Cubic Plus Association (CPA), while also a number of other software tools more accurately mirror contemporary conditions. However, these methods are still somewhat too demanding in time and computer resources to satisfy the everyday industrial user. But presentations by Michael Michelsen and several other CERE specialists clearly indicated that this situation is under rapid improvement.

### A steady inflow of graduates

Dr. Jim Bennett is a reservoir simulation specialist at consultancy company Schlumberger, which advices leading energy corporations around the globe on oil and gas recovery and related topics.

"In our work, we are entirely cubic, meaning that we rely on the cubic equations of state that have been in use in oil and gas industry for decades," Jim Bennett comments.

"However, this doesn't mean in any way that we don't trust the more advanced tools being developed by CERE and others. You can say that as consultants we are just following the market. Our priorities reflect what our clients are asking for."

Jim Bennett's own background is in mathematics:

"Thermodynamics is a field I have come to late in life. It is not absolutely essential to my daily work, but it is something I want to understand better. Michael Michelsen's course on thermodynamic modeling is where I can learn a lot; the Discussion Meeting is more of an overview."

Jim Bennett attends the event for his second consecutive year. Asked which ideas he brought home with him last year, the reply is:

"Well, first of all I suggested sending people to Michelsen's course. And I will make the same recommendation this year. At the same time, I have in mind not only to focus on the topics of the meeting. As a company we are also looking at people. Over recent years, Schlumberger has had a steady flow of graduates trained at the DTU, and the Discussion Meeting is a nice opportunity to get a picture of who are able to solve the kind of problems that are relevant to our business."

*Dr. Raghuraman Pitchumani brings several ideas home: I will take them into discussions with other groups at Shell.*

### Keen on equations

Dr. Graeme Keith of DONG Energy is on a similar note:

"Following the research at CERE will put us in a better position when people present us with their ideas such as suggestions on which kind of technology to use."

At DONG Energy, Graeme Keith's job is in geophysics R & D, meaning that he is engaged in maximizing the information obtainable from the vast amounts of seismic and similar data mainly about the geological structures in the Danish part of the North Sea. Having joined the company by January 2012 and having previously worked outside the energy resource engineering industry, he is a newcomer to the Discussion meeting.

"My first-hand impression is that the projects at CERE are highly relevant to a company like ours. I would say that if just, say, 10 percent of the projects here turn out successfully, and a few of the ideas later are used in full scale, it could have significant economic implications and prove to be a sound investment to the Danish society and the companies involved."

Holding a PhD. in mathematics and a post doc in applied mathematics, Graeme Keith found himself well at home at the Discussion Meeting:

"What I like about this conference is that people are not afraid of putting a bunch of equations up there. Not often will you find a collection of people with such a wide variety of backgrounds and fields, and still see that they are actually going in-depth on the various subjects. The technical engagement of the presenters means we get a great deal of insight in a wide range of themes. The rate of transfer of information is enormous!"

PhD defense

# Heterogeneously Catalyzed Chemical Reactions in Carbon Dioxide Medium

PHOTO: ALSU KHUSAINOVA

Nikolai E. Musko, PhD • Supervisors: Georgios Kontogeorgis, Jan-Dierk Grunwaldt, Anker Degn Jensen.

*The project was supported by the Danish Council for Independent Research: Technology and Production Sciences (FTP)*

In recent years it has become clear that carbon dioxide, $CO_2$, is a highly interesting medium in relation to a number of catalyzed chemical reactions in the fine chemicals industry and similar contexts. Of special interest is the super-critical state of $CO_2$, a range of temperature and pressure where $CO_2$ exhibits both liquid and gas-like behavior. Moreover, this behavior can be controlled, meaning that relatively small changes in temperature and/or pressure can result in quite dramatic changes in process conditions, which if applied correctly can be highly beneficial to the desired output.

In this project, production of dimethyl carbonate and propylene carbonate is studied closely. Both substances are of extremely high importance in the chemical industry.

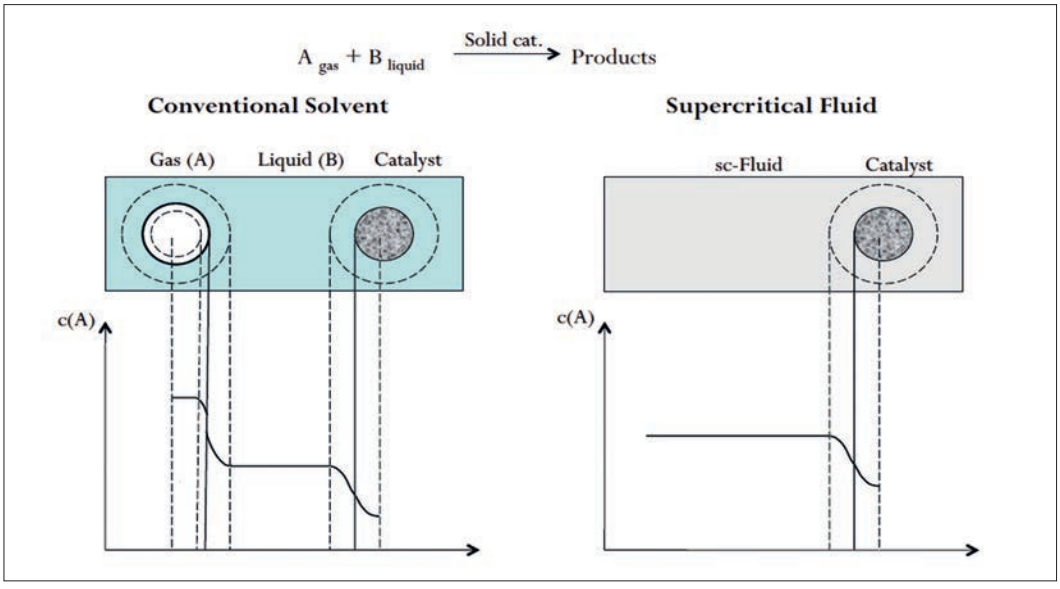
Many substances have the ability to exist at a super-critical state, meaning that at a given temperature and pressure the difference between gas and liquid phases disappears.

Super-critical fluids possess values of density similar to liquids. By changing the density of the fluid, its dissolution power can also be changed dramatically. This makes super-critical fluids attractive and effective solvents and reaction medium for many processes. On the other hand, some properties of super-critical fluids resemble those for gasses. For instance, dynamic and kinetic viscosities are normally lower than for the gaseous state, whereas diffusivity coefficients lie between those for gasses and liquids.

Under near-critical conditions, the substance will exhibit both liquid and gas-like behavior, and a slight change in temperature and/or pressure may cause either liquid or gas-like behavior to be more or less dominant.

$CO_2$ is one common substance with the ability to exist in super-critical state. It is cheap, non-toxic, relatively easy to handle, and has several other practical advantages. $CO_2$ has been used in numerous reactions, including homogeneous catalysis, bio-catalysis and heterogeneous catalysis. Almost all studies have shown that the use of $CO_2$ improves conversion and selectivity of the reactions. Further, in relation to the products studied in the project (dimethyl carbonate and propylene carbonate) $CO_2$ is able to not only act as a medium but also as a reactant which adds to the relevance of the reactions investigated.

In the project, the Cubic-Plus-Association Equation of State (CPA) was applied to heterogeneously catalyzed chemical reactions in $CO_2$ medium. It is shown that CPA is a powerful and universal model for predicting phase equilibria during direct synthesis of dimethyl carbonate from methanol and $CO_2$. It gives quite satisfactory results for low- and high-pressure vapor-liquid and liquid-liquid equilibria of the binaries and ternaries comprising the reaction mixture. Furthermore, CPA was successfully validated by the predicted bubble point pressure curves of quaternary mixtures that matched the experimental data closely.




*Super-critical fluids possess values of density similar to liquids. By changing the density of the fluid, its dissolution power can be changed dramatically. The illustration shows the difference in principle between a catalyzed reaction involving a conventional solvent versus a supercritical fluid.*

*Amino acid salt solutions have emerged as an alternative to traditional carbon dioxide capture techniques. Benedicte Mai Lerche's PhD. Defense on the subject attracted well deserved attention.*

PhD defense

# $CO_2$ Capture from Flue Gas using Amino Acid Salt Solutions

$CO_2$ capture has the potential for large reductions of $CO_2$ emissions from fossil fuel power plants. It is estimated that $CO_2$ capture may reduce emissions by as much as 80-90 per cent. The project investigates a relatively new technique for $CO_2$ capture using amino acid salt solutions.

Presently, available solvents for $CO_2$ capture are almost exclusively based on aqueous alkanolamine solutions. Alkanolamines are combinations of alcohols and ammonia. Most commonly used is MEA (monoethanolamine). However, the use of alkanolamines is known to have certain drawbacks. Firstly, the energy consumption in the present versions of the technique is quite high. This will increase electricity prices. Secondly, the conditions present during carbon dioxide capture from a power station's flue gas lead to some degree of alkanolamine decomposition. For one thing this is undesired simply because one loses solvent which in turn adds to costs. Worse, however, is the fact that some of the decomposition products are quite chemically reactive and may be harmful to human health.

Because the desire to capture $CO_2$ from flue gas is gaining momentum, there is an urgent need for the development of new solvents that have the ability to capture $CO_2$ in both a cost efficient and environmentally safe manner.

Amino acid salt solutions have emerged as an alternative. Amino acid based carbon capture can be described as a bio-mimetic process as it resembles the way carbon dioxide is captured by haemoglobin and other proteins in our blood. Amino acids may be produced synthetically or by fermentation or by hydrolyses of natural proteins.

Amino acids have the same amine functionality as alkanolamines, and alkaline amino acid salt solutions are expected to behave similarly towards $CO_2$ in flue gas and have several advantages. Their ionic nature makes them more stable to oxidative degradation and also gives them certain other desirable properties such as low volatility and high surface tension. A further advantage can be achieved by the interesting feature of several amino acid salt solutions to form solid precipitates when absorbing $CO_2$. Due to this phenomenon, the driving force for absorption can be maintained at a high level even at high $CO_2$ loadings. In addition, some amino acid salt solutions have been shown to react with $CO_2$ with reaction kinetics faster than MEA.

In the project, an evaluation of selected amino acid salt solutions in $CO_2$ capture was performed. Reaction kinetics, $CO_2$ loading capacity, and precipitation ability were studied in laboratory scale experiments.

Benedicte Mai Lerche, PhD. • Supervisors Kaj Thomsen and Erling H. Stenby

PhD defense

# Enhanced Oil Recovery with Surfactant Flooding

Sara Bülow Sandersen, PhD.
• Supervisors: Nicolas von Solms, Erling H. Stenby

The demand for oil is increasing, and as significant amounts of crude oil remain trapped inside reservoirs, research in Enhanced Oil Recovery (EOR) is growing. Surfactant flooding is an EOR technique in which the phase behavior inside the reservoir is manipulated by injection of surfactants and co-surfactants, creating advantageous conditions for mobilizing trapped oil. In this project, production of dimethyl carbonate and propylene carbonate is studied closely. Both substances are of extremely high importance in the chemical industry.

Correctly designed surfactant systems will result in micro-emulsions being formed at the interface between crude oil and water, reducing the interfacial tension (IFT) to ultra-low values, mobilizing the residual oil and thus improving oil recovery.

However, several challenges are associated with the technique, such as the adsorption of surfactants to the rock during the injection; chromatographic separation of the surfactants in the reservoir; and whether surfactants are resistant to and remain active at reservoir conditions such as high temperatures, pressures and salinities.

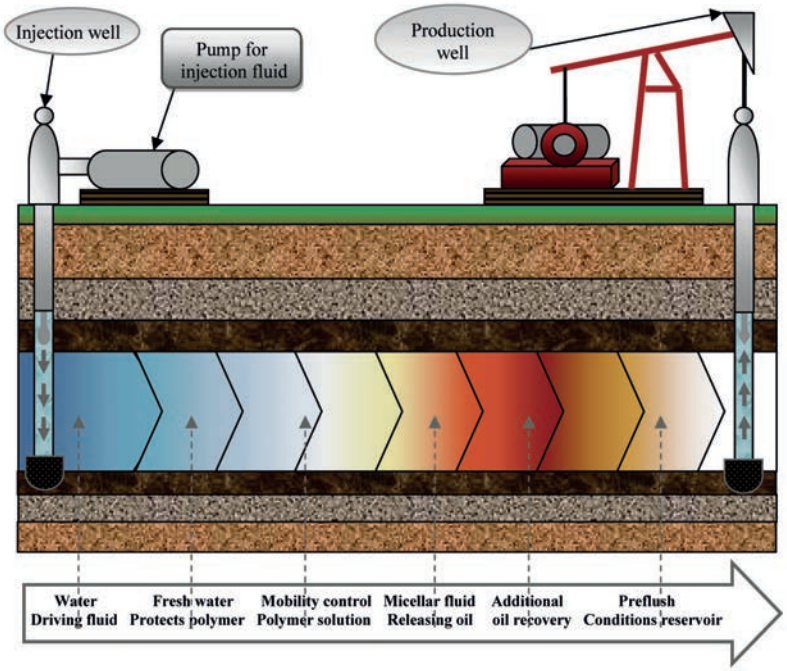
Correct modeling of phase behavior is essential in order to achieve the optimal surfactant flood design. In the project, a model surfactant system – water/NaCl/SDS/1-butanol/heptane – was studied at elevated pressures and a range of temperatures. It was seen that pressure had a significant influence on phase behavior. The trend was even more pronounced when an increase in temperature was added.

Further, a study of oil/brine systems was performed with oil and different brine solutions, where the brine solutions were modified by changing the sulfate concentration. A North Sea crude, a Latin American crude, a Middle East crude, and pure heptane were studied in a PVT cell. A significant decrease in the viscosity of the Latin American crude was measured after contacting with brine at high pressures. The viscosity decrease was more pronounced with increasing sulfate concentration in the brine. It is suggested that the viscosity decrease is explained by changes of the shape of the heavy component molecules present in the crude oil. It seems reasonable to suggest that sulfate and other ions influence the shape of the heavy components, which has been observed similarly for polymer studies. As the viscosity decrease is only observed for the Latin American crude oil, this seems reasonable when considering that the asphaltene content is three times higher for this oil than for the Middle East crude.

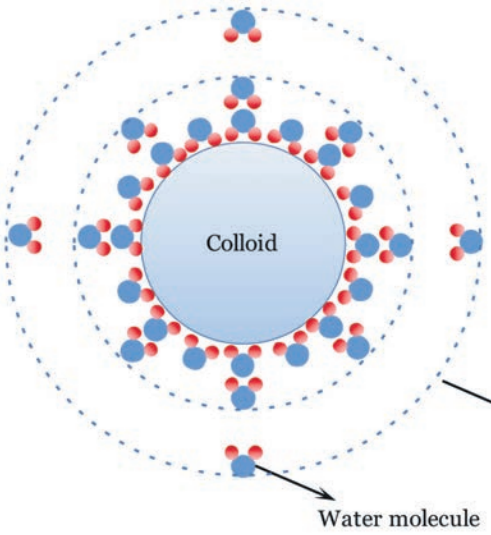
A second main conclusion is that the Middle East crude formed emulsions at high sulfate concentrations, elevated pressures, and elevated temperatures. The SARA analysis revealed that the Middle East crude oil has a large proportion of lighter components, and the GC analysis confirmed that the amount of light hydrocarbons changed significantly after the Middle East crude oil was contacted with brine in the PVT cell at elevated temperatures and pressures. It is suggested that the formation of emulsions is related to the presence of lighter hydrocarbons in the Middle East crude oil.

It is desirable to develop thermodynamic models capable of accurate phase behavior modeling of such complex systems. In the project, a modeling study with the sPC-SAFT equation of state model was carried out. It was shown that introducing a small binary interaction parameter fitted to each individual binary system results in good correlations.

*The project was supported by the Danish Council for Independent Research: Technology and Production Sciences (FTP)*




*The illustration presents a possible design for a process which introduces surfactant flooding in oil recovery.*




*Most colloidal interactions in nature take place under the presence of water molecules, which exhibit mutual hydrogen bonding. Hydrophobic colloids tend to aggregate in the aqueous phase. The water molecules are ordered around them. The ordered water molecules can be regarded as hydration shells radially propagating and decaying from the particle surface.*

PhD defense

# Particles in Pores – Stochastic Modeling of Polydisperse Transport

Hao Yuan, PhD.
• Supervisors: Alexander Shapiro, Erling H. Stenby

Colloids are particles dispersed in liquids with sizes in between dissolved macromolecules and suspended particles that resist rapid sedimentation. Colloid flow, filtration, and migration in porous media are widely observed in a number of important natural and industrial processes. Two examples relevant to the oil industry are mud filtration in drilling wells and injectivity decline during water injection.

The typical size of colloid particles ranges from 10 nano-meters to 10 micro-meters. Colloids in nature include mineral fragments, microbes, and plant decay debris. The mineral fragments, such as silicate clay, are mainly derived from soil and formation rocks.

The project aims at a better understanding of the transport of colloids in porous media. In oil and gas exploration, deposition and migration of colloids may cause permeability damage which subsequently leads to injectivity decline and productivity decline. Colloid transport is also highly relevant in microbial enhanced oil recovery (MEOR) where bacteria producing surfactants are injected in order to enhance oil production. Besides oil industry applications, understanding colloid transport may also be relevant in relation to e.g. the spreading of bacteria in aquifers and deep bed filtration during waste water treatment.

Fundamental filtration theory is focused on different scales: the interface scale, the collector (median grain) scale, and the pore scale. In all states, it is important to account for the fact that the particles and pores may be of different sizes. Moreover, the particles may have different residence times in the different pores. The classical filtration models do not account for these size and time distributions. Recent developments in this direction have not yet been made ready for practical applications.

In the project, a new mathematical model for colloid flow in porous media was developed. The model accounts for the particle and pore size distributions, as well as variation of the particle residence times. Several effects are discussed and explained, like sharp or non-monotonous particle deposition, or deep penetration of the relatively large particles.

The model has been applied to studying water injectivity decline under water flooding of petroleum reservoirs. The produced software accounts for the reservoir heterogeneity, two-phase flow (oil and water) and the distribution of solid particles by sizes. It also accounts for the later formation of the external filter cake and its erosion. The model is able to capture the behavior of the injectors in the field: the initial slow injectivity due to the build-up of the external cake, and the steady state during cake erosion. A software tool with a user-friendly interface was developed.

Another application of the filtration theory considered in the project was a method for improved oil recovery due to mobilization and relocation of the reservoir fines. Modeling of this effect in a layer-cake reservoir was carried out.

PhD defense

# Smart Water Flooding in Carbonate Reservoirs

Adeel Zahid, PhD.
• Supervisors: Alexander Shapiro, Erling H. Stenby, Wei Yan

Injection of water has been used in oil and gas recovery for decades. It was first practiced for pressure maintenance after primary depletion and has since become the technique most widely applied in order to improve oil recovery. Recent findings suggest that changing salinity or making other modifications to the injected water may increase yields further. The aim of the project is to improve the understanding of the mechanisms involved in this type of "smart" water flooding.

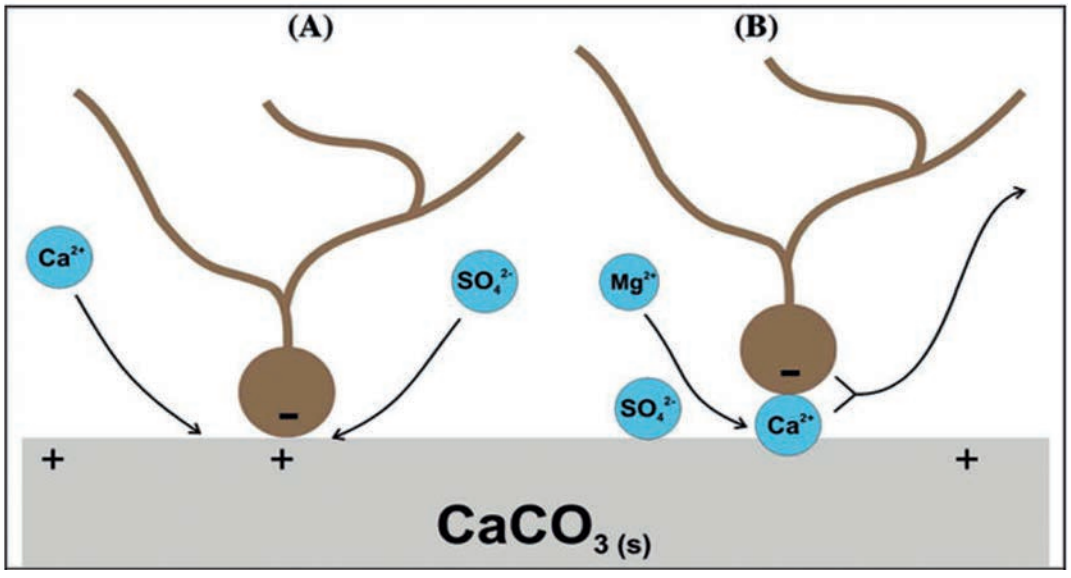
Traditionally, the role of chemistry in injection water on displacement efficiency or its impact on oil recovery has been given little attention in reservoir engineering practice. However, over the last decade extensive studies have shown that composition of injected water can affect crude oil / brine / rock interactions. Low salinity water flooding in sandstone reservoirs is now a mature technology; high salinity, high temperature flooding in chalk rock has also been investigated. Recently, low salinity water flooding has also been applied to carbonates.

In this study the potential of advanced water flooding is studied throug experiments with reservoir chalk samples with special attention given to potential determining ions, which are the ions mostly affecting the fluid-rock interactions. Two different water flooding schemes – with and without aging – were used for North Sea reservoir samples. For comparison, tests were carried out with Stevns Klint core plugs. The brines with different concentrations of sulphate and magnesium ions were injected under varying temperature.

The study yielded five main findings. Firstly, injection of sulphate rich brine may lead to additional recovery from Stevns Klint chalk even under completely water wet conditions – therefore, increment in oil recovery with sulphate ions cannot be explained just by the rock wettability alteration. Secondly, sulphate ions may help decrease the crude oil viscosity when brine is contacted with oil under high temperature and pressure; for other oils this contact may result in formation of stable emulsions. Thirdly, viscosity reduction for crude oil in contact with brine is connected to the presence of heavy components in the crude oil, while formation of emulsions with brine is a phenomenon related to the presence of lighter components in the crude oil. Further, the reservoir chalk rocks showed relatively less effect of temperature and sulphate ions concentration on oil recovery as compared to Stevns Klint outcrop chalk – this indicates that the rock may also determine whether the effect of temperature and high salinity brine on the recovery is observed. And finally, migration of fines and dissolution of rock particles are possible mechanisms of oil recovery increment with low salinity brines from carbonate core plugs at 90 degrees °C.

While the project has made a contribution to the understanding of smart water flooding, the experimental data on alternating salinity water flooding in carbonates remain limited, leaving scope for further experiments and mechanistic studies.

*The project was funded by DONG Energy and The Danish Council for Independent Research / Technology and Production Sciences (FTP) as part of the ADORE project.*




*Schematic model of the wettability alteration induced by sea water. Figure (A) shows the proposed mechanism when $Ca^{2+}$ and $SO_4^{2-}$ are active. Figure (B) shows the proposed mechanism when $Mg^{2+}$ and $SO_4^{2-}$ are active.*

# More Strength within Rock Mechanics

Filling a newly created position as Assistant Professor at DTU Civil Engineering, PhD Katrine Alling Andreassen enhances the scope of CERE's geotechnical and rock mechanical activities. She has investigated rock mechanical properties of chalk through the last decade with several subjects of high relevance to oil and gas recovery.

Since defending her PhD thesis in May 2011, Katrine Alling Andreassen has worked as an engineering consultant with Ramboll until taking on the position at DTU by June 1st, 2012. The time with Ramboll has allowed Katrine Alling Andreassen to gain experience with practical engineering problems related to geotechnics and rock mechanics such as the early preparations for the construction of the Fehmern Belt tunnel to connect the Danish island of Lolland to Germany, and the ground investigation for concrete foundations for large scale wind turbines off the shore of England.

In her PhD project entitled *Temperature Influence on Rock Mechanical Properties* she investigated how changes in temperature and fluids affect strength and deformation behavior of chalk. The findings are of high relevance to Enhanced Oil Recovery (EOR). Besides experiments, the project created an extensive database encompassing results from more than 600 laboratory experiments published on the subject. In her new position, Katrine Alling Andreassen will continue these activities while also taking on activities related to other geological fields including shale, clay, and sandstone.

*Katrine Alling Andreassen increases the scope of CERE's geotechnical and rock mechanical activities of relevance to Enhanced Oil Recovery in chalk. She will also take on activities in other fields including shale, clay, and sandstone.*

# Bringing a US flavor to CERE

Albeit born and raised in Denmark and trained at DTU Chemical Engineering, Associate Professor Kristian Jessen brings an American touch to CERE. On leave from his position as Associate Professor at the University of Southern California, he fills a position as Visiting Faculty at DTU Chemical Engineering. The arrangement is in place until summer 2013.

Kristian Jessen's research addresses a number of CERE's core areas including modeling and simulation of Enhanced Oil Recovery (EOR); $CO_2$ sequestration; recovery of non-conventional resources including production of natural gas from shale; oil recovery from low-permeable source rocks; and combinations of these – including the co-optimization of $CO_2$ EOR and $CO_2$-sequestration. A key component of his research activities relates to the development, validation, and implementation of accurate physical models in engineering simulation tools.

*On leave from his position as Associate Professor at the University of Southern California, Kristian Jessen fills a position as Visiting Faculty at DTU Chemical Engineering.*

After obtaining his PhD degree at DTU Chemical Engineering in 2001, Kristian Jessen worked a Research Associate and Acting Faculty at the Department of Petroleum Engineering at Stanford University, USA, until moving on to the University of Southern California in 2006.

# The French Connection(s) visit CERE

Over the recent years, cooperation between CERE and the Thermodynamic Laboratory of the Ecole de Mines de Paris has grown steadily stronger. During autumn 2012, one of the laboratory's founding fathers, Dr. Dominique Richon, as well as it's current head, Dr. Christophe Coquelet, lectured at DTU.

Dr. Richon, now retired, is author or co-author of 15 patents and more than 300 papers in peer reviewed journals. At August 30th, he gave a presentation on "Experimental Thermodynamics for Chemical Process Engineering" in his capacity as Otto Mønsted Visiting Professor at the Department of Chemical and Biochemical Engineering, DTU.

Dr. Coquelet visited CERE on October 25th having headed the Thermodynamic Laboratory of the Ecole de Mines de Paris since 2009. Under the title "Presentation of the CEP TEP laboratory: new Center of Thermodynamic of Processes", he introduced the current scope of the laboratory which in 2013 will be transformed into Center of Thermodynamic of Processes (CTP).

*From the visit of Dr. Dominique Richon (left) at CERE, August 2012.*

# A US view on colloids

The transport of tiny particles known as colloids is not accurately described by traditional theories, according to Dr. Scott Bradford of the USDA; ARS, Salinity Laboratory in Riverside, California. At November 8th, 2012, Dr. Bradford lectured at DTU on "Colloids in the Subsurface: Applications, Theory and Challenges". According to Scott Bradford, factors such as the influence of pore space geometry, system hydrodynamics, colloid concentration, aggregation, surface macromolecules, and ion exchange have been neglected in classical retention models. Transport of colloids in porous media is of relevance to a number of applications including the transport and fate of microorganisms, contaminants, and nano-particles in soil and groundwater environments.

*CERE administrative staff. From left Christian Carlsson, Rune Andersen, Patricia Wagner, Anne Louise Biede.*

# A tight-knit Unit

The small administrative staff are seasoned veterans in the art of supporting an efficient and ambitious research organization like CERE.

A dedicated unit of only four people keeps CERE's administrative engine up and running. They do not act on there own, of course, but it is these four who deal with the daily nitty-gritty of running a professional research group with more than 60 scientists, PhDs and postdocs.

Born in Paris and having moved to Denmark six years ago, Project Administrator Patricia Wagner sums up the task facing the small administrative unit of CERE:

"Our scientists are extremely creative and driven people. Their focus is so strong that everyday practicalities are better handled by us leaving them to do what they do best: research and innovative thinking."

Secretary Anne Louise Biede shares the view on the administrative unit's responsibilities and key role in the scientific process:

"We pride ourselves of our ability to foresee and fix potential administrative problems facing the scientists and students before they become issues." And often the experience and professionalism of the tight-knit unit creates an illusion of a hidden crystal ball warning the team of large and small problems looming in the horizon.

## Explaining Denmark

When foreign PhD students and other non-Danish staff join CERE, Patricia is usually the one "explaining Denmark to them" as she puts it. Having moved to Denmark recently she is well suited as gatekeeper and guide to EU regulations and local laws.

Christian has worked with CERE since 1997. As Systems Administrator he takes care of administrative infrastructure, IT systems, and logistics. It is also Christian who delivers photo and video documentation of scientific experiments, and CERE events.

"Quite often I head home with a feeling that I didn't get to do any of the things I had scheduled for that day. But that's ok. After all, it's our job to eliminate the problems that the scientific staff faces" he explains.

Still, Christian cannot claim seniority, although he's been around for 15 years. Known as Louise to everybody, Anne Louise Biede has been with DTU Chemical Engineering since 1993. In relation to CERE, only Director Erling Stenby and Professor Michael Michelsen can match her seniority. It is Louise that the foreign students and PhDs turn to if the loneliness becomes too much.

"We are replacing parents at times", Louise explains.

"More than once have I entered an office to find a young PhD student there who is so preoccupied by work that he or she is forgetting simple everyday details like three square meals or warm clothing when the snow is piling

*...to be continued*

up outside". Patricia agrees with Louise's account of the young talents life far away from home:

"They might receive a phone call that a close relative is sick – where can they go? Most likely they choose our office, and more than once we are able to send them back to the lab with a smile on the face. It's all about listening and caring."

The members of the administrative unit find that participating in events with the scientific staff is very motivating:

"It was never an issue whether we should be present at the annual Discussion Meeting or various excursions" Louise says, adding:

"This means that not only are we known by everybody in the staff, we also have good working relations with external partners and members of the industrial Consortium. We all take pride in supporting a smooth and professional operation."

*Laboratory manager Karin Petersen with colleagues (from left) Sinh Hy Nguyen, Duc Thoung Vu, Povl Valdemar Andersen, Hector Osvaldo Ampuero Diaz, Thoung Dang, Zacarias Tecle.*

# Experience and Creativity

CERE laboratory crew is a strong, innovative unit logging more than 175 years of accumulated experience with oil and gas research projects.

One of the cornerstones of the CERE research organization is the strong crew manning laboratories and building the laboratory equipment needed in the research projects. With an average of 25 years in the business, the team of 8 have logged more than 175 years of experience with research projects primarily related to the oil and gas industry. Laboratory Manager Karin Petersen is convinced that the respect and personal friendships that have grown within the group over the years are some of the main reasons for the efficiency and innovative power of the team.

"Our work has a strong creative element; we often have to invent new, technical solutions and build tailor-made equipment to meet the scientific objectives in the CERE projects. It is challenging but also one of the key reasons why we all love to work with CERE: it is a truly innovative environment with a lot of esprit, and as a team, we always have to give it our very best to solve the problems and reach our objectives in cooperation with the scientific staff. It is a very rewarding process," Karin Petersen says.

# A broader Scope

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

The NextOil DK program will allow CERE to assist oil and gas production from deep reservoirs in the Danish part of the North Sea. This was not the only new frontier opening to us in 2012.

CERE is a strong research center growing stronger with specialists covering most key areas in the diverse field of energy resource engineering. This year, together with our industrial partners from Maersk Oil, GEO, and DONG Energy we took the first step towards a new area of competences with the NextOil initiative looking into challenges of High Pressure, High Temperature oil and gas production. It is a complete new area of research supported by The Danish National Advanced Technology Foundation as well as the partners, and we very much look forward to sharing and discussing our findings with CERE members and partners in the years to come.

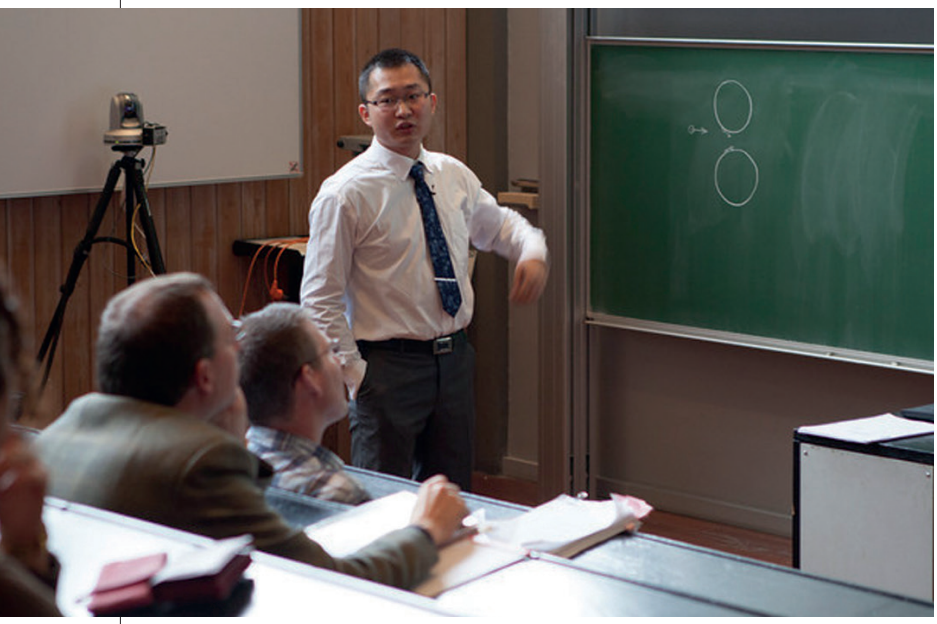
In 2011, we initiated two major research projects: BioRec (Biotechnology in Oil recovery) supported by The Danish National Advanced Technology Foundation, and SmartWater looking into novel water flooding techniques supported by EUDP. Both projects involve a number of industrial and academic partners; and both show good progress as reported on the previous pages. Also moving ahead at full speed are several projects within post-combustion CO2-capture and the projects "$CO_2$ Hydrates – Challenges and Possibilities" project (a joint project with Ecole des Mines in France); and "Calculating Dew Points for Natural Gas containing Water and/or selected Production Chemicals" are other examples of new projects. The latter project is sponsored by GERG which is The European Gas Research Group, and is related to CERE's well established CHIGP (Chemicals in Gas Processing) project. Completing its 10th consecutive year in 2012, this Joint Industry Project keeps producing valuable theoretical and experimental results. Having already several other industry Consortium members onboard, CHIGP was able to greet Petrobras as a new participant this year. On the same note, I am pleased to welcome Hess Corporation and Infochem as new members of the CERE Consortium.

## A small, flexible core

Obviously, the many new research projects have increased our activity, meaning that we have been able to greet many new faces, not least a number of new PhD students, visiting professors and other scientific personnel. However, we have managed to absorb the new activities while almost keeping the size of our faculty at the same level as last year.

This underlines a point in our strategy. Rather than aiming to grow CERE into a large, department-like structure, we prefer to enjoy the flexibility of having a small

*The 2012 version of CERE's annual Discussion Meeting, held at the Pharmakon conference center in Hillerød, had strong industry representation: 34 participants from 17 companies.*



*Hao Yuan's PhD defense of on colloid flow in porous media (see page 19).*

dedicated core while being able to establish cooperation with other DTU departments when relevant. Today we have faculty members and other scientific staff from DTU Chemical Engineering, DTU Space, DTU Compute, DTU Civil Engineering, and DTU Chemistry. Thus, our faculty covers a broad range of disciplines, ensuring that we will be able to set up cooperation smoothly across the DTU with the relevant expertise for a given project.

No rule without an exception, and this year we were able to welcome PhD Katrine Alling Andreassen as a new faculty. Filling a position as assistant professor at DTU Civil Engineering, she enhances the geological competences already secured by professor Ida L. Fabricius' group. Katrine Alling Andreassen has investigated rock mechanical properties of chalk during the last decade with several subjects of high relevance to oil and gas recovery. She will also take on activities in other fields including shale, clay, and sandstone.

*The geological competences of CERE were strengthened further in 2012. One key subject is rock mechanical properties of chalk which is of high relevance to oil and gas recovery in the North Sea.*

Representing another expansion of CERE's faculty, albeit temporary, is Kristian Jessen. On leave from his position as Associate Professor at the University of Southern California, he fills a position as Visiting Faculty at DTU Chemical Engineering. The arrangement is in place until summer 2013. Kristian Jessen's research addresses a number of CERE's core areas including modeling and simulation of Enhanced Oil Recovery (EOR); $CO_2$ sequestration; recovery of non-conventional resources including production of natural gas from shale; oil recovery from low-permeable source rocks; and combinations of these – including the co-optimization of $CO_2$ EOR and $CO_2$-sequestration.

## Successful trip to Houston

For everybody at CERE it was a much awaited event when professor Michael Michelsen, the centers grand old man, summed up experience gained over the past decade within calculation of phase equilibrium, a brilliant presentation that was followed by numerous questions from the audience.

I am happy to announce that Michael Michelsen will continue his involvement in CERE's activities. Amongst other projects, he will assist senior scientist Wei Yan in the further development of multiphase flash reservoir simulations.

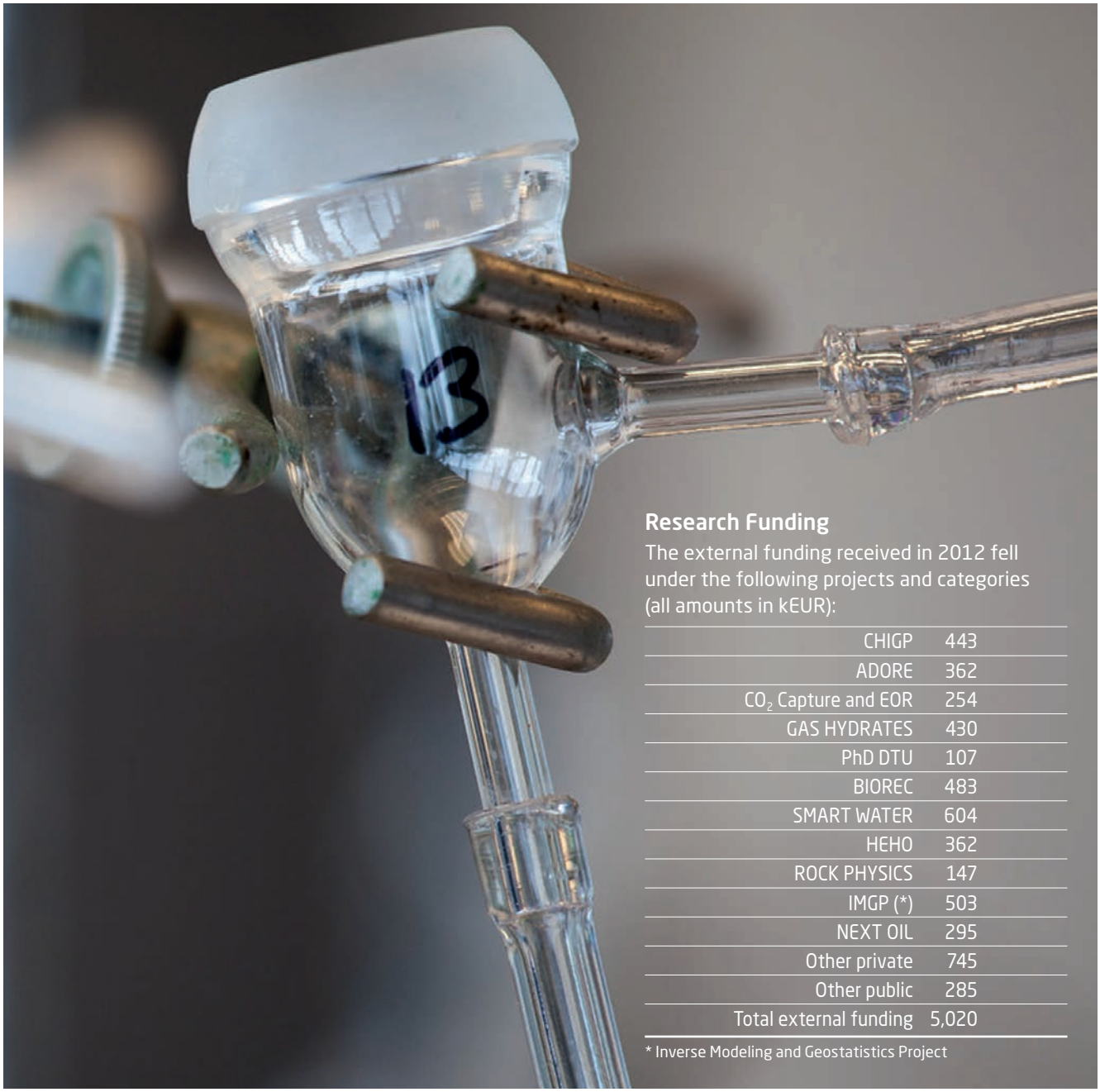
A special event in 2012 was our trip to Houston in March. No less than 45 CERE staff members, reaching across a wide range of disciplines and functions, took part in the excursion. The high degree of participation was impressive in itself and was fully matched by the hospitality of the many US companies and academic institutions which were kind enough to open their doors and spend time with us. For that we are truly grateful.

Naturally, I am not able to comment on all activities of the year within the limitations of this text. If you have any inquiries to the above or to items not covered here, please feel free to contact me.

# Research Funding

As a university research center, our objective is to spend all of our money on research. No 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 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 2012, our external funding increased significantly to a total budget of EUR 5.0 million.



**Research Funding**

The external funding received in 2012 fell under the following projects and categories (all amounts in kEUR):

| | |
|---|---|
| CHIGP | 443 |
| ADORE | 362 |
| $CO_2$ Capture and EOR | 254 |
| GAS HYDRATES | 430 |
| PhD DTU | 107 |
| BIOREC | 483 |
| SMART WATER | 604 |
| HEHO | 362 |
| ROCK PHYSICS | 147 |
| IMGP (*) | 503 |
| NEXT OIL | 295 |
| Other private | 745 |
| Other public | 285 |
| Total external funding | 5,020 |

* Inverse Modeling and Geostatistics Project

# Conference contributions & Invited speakers


## IEEE PES Conference on Innovative Smart Grid Technologies (ISGT): Washington, D.C, USA, 16-20 January, 2012

Halvgaard, R.; Poulsen, N. K.; Madsen, H.; Jørgensen, J.B. 2012: **"Economic Model Predictive Control for Building Climate Control in a Smart Grid"** (Oral presentation), IEEE PES Conference on Innovative Smart Grid Technologies (ISGT), Washington, D.C., January 16-20, 2012 Proceedings from 2012 IEEE PES Innovative Smart Grid Technologies (ISGT) (ISBN: 9781457721588), pages: 6175631 DOI: 10.1109/ISGT.2012.6175631

## Third EAGE Shale Workshop Shale Physics and Shale Chemistry: New Plays, New Science, New Possibilities, Barcelona, Spain 23-25 January 2012.

Fabricius, I. L., 2012: **"Pore Size and Permeability of Experimentally Compacted Smectite and Kaolinite Clay"**. (Oral presentation), Third EAGE Shale Workshop Shale Physics and Shale Chemistry: New Plays, New Science, New Possibilities, Barcelona, Spain, 23-25 January, 2012. Proceedings, 78-81.

Mbia, E. N.; Fabricius, I. L., 2012: **"Pore Radius and Permeability Prediction from Sonic Velocity"** (Oral presentation), Third EAGE Shale Workshop Shale Physics and Shale Chemistry: New Plays, New Science, New Possibilities, Barcelona, Spain, 23-25 January, 2012. Proceedings, 82-87.

## 17th Nordic Process Control Workshop, Kgs Lyngby, Denmark, 26 - 27 January 2012.

Boiroux, D.; Schmidt, S.; Duun-Henriksen, A.K.; Frøssing, L.; Nørgaard, K.; Madsbad, S.; Skyggebjerg, O.; Poulsen, N.K.; Madsen, H.; Jørgensen, J.B. 2012: **"Control of Blood Glucose for People with Type 1 Diabetes: an in Vivo Study"** (Oral presentation), 17th Nordic Process Control Workshop, Kongens Lyngby, Denmark, 26-27 January, 2012. Proceedings of the 17th Nordic Process Control Workshop (ISBN: 978-87-643-0946-1), pages: 133-140, 2012.

Boiroux, D.; Schmidt, S.; Duun-Henriksen, A.K.; Frøssing, L.; Nørgaard, K.; Madsbad, S.; Skyggebjerg, O.; Poulsen, N.K.; Madsen, H.; Jørgensen, J.B. 2012: **"Control of Blood Glucose for People with Type 1 Diabetes: an in Vivo Study"** (Sound/Visual production (digital) - Sound/Visual production (digital)), 17th Nordic Process Control Workshop, Kongens Lyngby, Denmark, 26-27 January, 2012.

Capolei, A.; Völcker, C.; Frydendall, J.; Jørgensen, J.B. 2012: **"Single Shooting and ESDIRK Methods for adjoint-based optimization of an oil reservoir"** (Oral presentation), 17th Nordic Process Control Workshop, Kongens Lyngby, Denmark, 26-27 January, 2012. Proceedings of the 17th Nordic Process Control Workshop (ISBN: 978-87-643-0946-1), 2012.

Capolei, A.; Völcker, C.; Frydendall, J.; Jørgensen, J.B. 2012: **"Single Shooting and ESDIRK Methods for adjoint-based optimization of an oil reservoir"** (Sound/Visual production (digital) - Sound/Visual production (digital)), 17th Nordic Process Control Workshop, Kongens Lyngby, Denmark, 26-27 January, 2012.

Gade-Nielsen, N. F.; Jørgensen, J.B.; Dammann, B. 2012: **"Iterative Methods for MPC on Graphical Processing Units"** (Oral presentation), 17th Nordic Process Control Workshop, Kongens Lyngby, Denmark, 26-27 January, 2012. Proceedings of the 17th Nordic Process Control Workshop (ISBN: 978-87-643-0946-1), pages: 161, 2012.

Engoulevent, F.G.; Jørgensen, J.B. 2012: **"Simulation, Control and Optimization of Single Cell Protein Production in a U-Loop Reactor"** (Oral presentation), 17th Nordic Process Control Workshop, Kongens Lyngby, Denmark, 26-27 January, 2012. Proceedings of the 17th Nordic Process Control Workshop (ISBN: 978-87-643-0946-1), pages: 203, 2012.

Halvgaard, R.; Poulsen, N.K.; Madsen, H.; Jørgensen, J.B. 2012: **"Modeling Smart Enery Systems for Model Predictive Control"** (Oral presentation), 17th Nordic Process Control Workshop, Kongens Lyngby, Denmark, January 26-27, 2012. Proceedings of the 17th Nordic Process Control Workshop (ISBN: 978-87-643-0946-1), pages: 175, 2012.

Sokoler, L.E.; Edlund, K.; Mølbak, T.; Poulsen, N.K.; Madsen, H.; Jørgensen, J.B. 2012:**"Stochastic Model Predictive Control with Applications in Smart Energy Systems"** (Oral presentation), 17th Nordic Process Control Workshop, Kongens Lyngby, Denmark, 26-27 January, 2012. Proceedings of the 17th Nordic Process Control Workshop (ISBN: 978-87-643-0946-1), pages: 206, 2012.

Standardi, L.; Edlund, K.; Poulsen, N.K.; Jørgensen, J.B. 2012: **"A Dantzig-Wolfe Decomposition Algorithm for Linear Economic MPC of a Power Plant Portfolio"** (Oral presentation), 17th Nordic Process Control Workshop, Kongens Lyngby, Denmark, 26-27 January, 2012. Proceedings of the 17th Nordic Process Control Workshop (ISBN: 978-87-643-0946-1), pages: 141, 2012.

Ohan, V.; Steinke, F.; Metzger, M.; Runkler, T.; Jørgensen, J.B. 2012: **"Model Predictive Control for an Industrial SAG Mill" (**Oral presentation) 17th Nordic Process Control Workshop, Kongens Lyngby, Denmark, 26-27 January, 2012. Proceedings of the 17th Nordic Process Control Workshop (ISBN: 978-87-643-0946-1), pages: 208, 2012.

Lerch, D.M.; Völcker, C.; Capolei, A.; Jørgensen, J.B.; Stenby, E.H. 2012: **"Optimisation of Oil Production in Two - Phase Flow Reservoir Using Simultaneous Method and Interior Point Optimiser"** (Oral presentation),17th Nordic Process Control Workshop, Kongens Lyngby, Denmark, 26-27 January, 2012. Proceedings of the 17th Nordic Process Control Workshop (ISBN: 978-87-643-0946-1), pages: 191, 2012.

Zhou, G.; Huusom, J.K.; Jørgensen, J.B. 2012**:"State Estimation for the Automotive SCR Process"** (Oral presentation), 17th Nordic Process Control Workshop, Kongens Lyngby, Denmark, 26-27 January, 2012. Proceedings of the 17th Nordic Process Control Workshop (ISBN: 978-87-643-0946-1), pages: 204, 2012

Völcker, C.; Jørgensen, J.B.; Thomsen, P.G.; Stenby, E.H. 2012: **"Production Optimization for Two-Phase Flow in an Oil Reservoir"** (Oral presentation), 17th Nordic Process Control Workshop, Kongens Lyngby, Denmark, 26-27 January, 2012. Proceedings of the 17th Nordic Process Control Workshop (ISBN: 978-87-643-0946-1), pages: 198, 2012.

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### Thirty-Seventh Workshop on Geothermal Reservoir Engineering, California, USA, 30 January - 1 February 2012.

Rosenbrand, E.; Fabricius, I.L.; Shapiro, Yuan, H. 2012: **"Thermally induced permeability reduction due to particle migration in sandstones: the effect of temperature on kaolinite mobilization and aggregation"** (Oral presentation), Thirty-Seventh Workshop on Geothermal Reservoir Engineering, California, USA, 30 January - 1 February, 2012

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### IEEE International Electric Vehicle Conference (IEVC), Greenville, SC, USA, 4 - 8 March 2012.

Halvgaard, R.; Poulsen, N.K.; Madsen, H.; Jørgensen, J.B.; Marra, F.; Bondy, D.E.M. 2012: **"Electric vehicle charge planning using Economic Model Predictive Control"** (Oral presentation), 2012 IEEE International Electric Vehicle Conference (IEVC), Greenville, SC, 4-8 March, 2012. Proceedings from 2012 IEEE International Electric Vehicle Conference (IEVC) (ISBN: 9781467315623), 2012, DOI: 10.1109/IEVC.2012.6183173

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### InMoTher - Industrial Use of Molecular Thermodynamics, LYON, France, 19-20 March, 2012

Mustaffa, A.A.; Kontogeorgis, G.; Gani, R. 2012: **"Application of the UNIFAC-CI Model for Phase Equilibria Predictions of Organic Chemical System"** (Poster presentation), InMoTher 2012, Lyon, France, 19-20 March 2012.

Tsivintzelis I., Michelsen M.L., Stenby E.H., Kontogeorgis G.M. 2012: **"Application of CPA to Mixtures Containing Acid Gases"** (Poster Presentation), Industrial Use of Molecular Thermodynamics - InMoTher 2012, Lyon, France, 19-20 March 2012. Conference proceedings electronic edition, InMoTher 2012, Lyon-France, 29-20/3/2012.

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### University of Houston, USA, 23 March, 2012

Fabricius, I. 2012: **"Static and Dynamic Effective Stress Coefficient of Chalk"**, (Invited Oral presentation), University of Houston, USA, 23 March, 2012

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### 18th SPE Improved Oil Recovery Symposium, Tulsa, Oklahoma, USA, 14-18 April 2012

Yan, W.; Michelsen, M.L.; Stenby, E.H. 2012 **"Calculation of Minimum Miscibility Pressure using Fast Slimtube Simulation"** (Oral presentation), 18th SPE Improved Oil Recovery Symposium, Tulsa, Oklahoma, USA, 14-18 April 2012

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### SPE EOR Conference at Oil and Gas West Asia, Muscat, Oman, 16 - 18 April 2012.

Zahid, A.; Shapiro, A.A.; Skauge, A. 2012: **"Experimental studies of low salinity water flooding in carbonate reservoirs: A new promising approach"** (Oral presenta-

tion), SPE EOR Conference at Oil and Gas West Asia, Muscat, Oman, 16-18 April, 2012. SPE paper 155625

### East Meets West Krakow International Student Congress, Krakow, Poland, 25-27 April, 2012

Lerch D; Capolei A.;Völcker C. J.B. Jørgensen; Stenby E.H. **"Simulation and Optimization of Oil Production under Waterflooding of the Two-Phase Flow Reservoir Using Simultaneous Method and Interior Point Optimiser."** (Oral Presentation), East Meets West Krakow International Student Congress (AGH Science University of Technology), Poland, Krakow, 25-27, April, 2012.


### International Conference of Porous Media, Indiana, USA, 14-16 May, 2012

Yuan, H.; Shapiro A.A.; You, Z.; Bedrikovetsky, P. 2012: **"Percolation of particles in pores"** (Oral presentation), International Conference of Porous Media, Indiana, USA, 14-16 May, 2012

### 2012 IFAC Workshop, Trondheim, Norway, 31 May-1 June 2012

Capolei, A.; Völcker, C.; Frydendall, J.; Jørgensen, J.B. 2012: **"Oil Reservoir Production Optimization using Single Shooting and ESDIRK Methods"** (Oral presentation), 2012 IFAC Workshop, Trondheim, Norway, 31 May-1 June, 2012. Proceedings from Automatic Control in Offshore Oil and Gas Production (ISBN: 978-3-902661-99-9), pages: 286-291, 2012, DOI: 10.3182/20120531-2-NO-4020.00030

### Fjernvarmens fossilfrie fremtid, Copenhagen, Denmark, 30 May, 2012

Fabricius, I. 2012: **"Varmelagring i Danmarks dybe undergrund", (Invited Oral Presentation),** Fjernvarmens fossilfrie fremtid, Copenhagen, Denmark, 30 May, 2012

### Applied Molecular Simulations for Product and Process Design, Paris, France, 31 May-1 June, 2012.

Kontogeorgis, G.M. 2012: **"Association models for applications in the petroleum and chemical industries"** (Invited presentation), SciMeeting 2012, Applied Molecular Simulations for Product and Process Design, Paris, France, 31 May-1 June, 2012.


### 74th EAGE Conference & Exhibition incorporating SPE EUROPEC, Denmark, 4-7 June 2012

Alam, M. M.; Hjuler, M.L.; Christensen, H.F.; Fabricius, I. L., 2012: **"Change of Static and Dynamic Elastic Properties due to $CO_2$ Injection in North Sea Chalk"**. (Oral presentation), 74th EAGE Conference and Exhibition incorporating SPE EUROPEC, Copenhagen, Denmark, 4-7 June, 2012. Paper D047, 4 pp.

Awadalkarim, A.; Fabricius, I. L., 2012: **"The Influence of Biot's Coefficient on the Estimation of Effective Stress on Deep Sea Sediments"**. (Poster presentation), 74th EAGE Conference and Exhibition incorporating SPE EUROPEC, Copenhagen, Denmark, 4-7 June, 2012. Paper P187, 4 pp.

Fabricius, I. L., 2012**: "Chalk as a reservoir":** (Invited Oral presentation), 74th EAGE Conference and Exhibition incorporating SPE EUROPEC, Copenhagen, Denmark, 2012, 4-7 June, 2012. Workshop on Chalk. 1p.

Hansen, T.M.; Cordua K.S.; Mosegaard, K. 2012: **"The role of geostatistics as prior information for solving inverse problems"** (Oral presentation), 74th EAGE Conference and Exhibition incorporating SPE EUROPEC, Copenhagen, Denmark, 4-7 June, 2012. Workshop on "integration of information from different sources", co-convened with Dr. Klaus Mosegaard, Copenhagen, Denmark, 4-7 June, 2012

Hansen, T.M.; Cordua K.S.; Mosegaard, K. 2012: **"Multiple scenario inversion of reflection seismic prestack data"** (Oral presentation), EAGE 2012 74th EAGE Conference and Exhibition incorporating SPE EUROPEC, Copenhagen, Denmark, 4-7 June, 2012., Copenhagen, Denmark, 4-7 June, 2012

Hedegaard, K. , Fabricius, I. L.;, 2012: **"Effect of Fluid Dynamic Viscosity on the Strength of Chalk".** (Poster presentation), 74th EAGE Conference and Exhibition incorporating SPE EUROPEC, Copenhagen, Denmark, 4-7 June, 2012. Paper p311. 4 pp.

Mbia, E. N., Fabricius, I. L., and Krogsbøll, A. 2012: **"Different Methods of Predicting Permeability in Shale"** (Poster presentation) 74th EAGE Conference & Exhibition incorporating SPE EUROPEC, Copenhagen, Denmark, 4-7 June 2012. Paper P186, 4pp.

Melnikova Y., Lange K., Frydendall J., Mosegaard K. 2012: **"A novel approach for combining multiple-point statistics and production data in reservoir characterization"** (Oral presentation), 74th EAGE Conference & Exhibition, incorporating SPE EUROPEC, Copenhagen,

4-7 June, 2012. Proceedings of the 74th EAGE Conference & Exhibition, Copenhagen, 2012.

Michelsen, M.L.; Yan, W.; Stenby, E.H. 2012 **"A Comparative Study of Reduced Variables Based Flash and Conventional Flash"** (Oral presentation), 74th EAGE Conference & Exhibition incorporating SPE EUROPEC, Copenhagen, 4-7 June, 2012

Rosenbrand, E.; Fabricius, I. L., 2012: **"Effect of Hot Water Injection on Sandstone Permeability - An Analysis of Experimental Literature".** (SPE 154489). (Oral presentation), 74th EAGE Conference and Exhibition incorporating SPE EUROPEC, Copenhagen, Denmark, 4-7 June, 2012. 11pp.

Sørensen, M. K.; Fabricius, I. L., 2012:**"Determining Upper Bounds for the Clay-squirt Effect in Clay Bearing Sandstone"**. (Oral presentation), 74th EAGE Conference and Exhibition incorporating SPE EUROPEC, Copenhagen, Denmark, 4-7 June, 2012. Paper I005, 4pp.

Yuan, H.; Nielsen, S.M.; Shapiro, A.A.; Bedrikovetsky, P. 2012: **"A new comprehensive approach for predicting injectivity decline during waterflooding"** (Oral presentation), SPE Europec/EAGE Annual Conference, Copenhagen, Denmark, 4-7 June, 2012. SPE paper 154509

### 82th Ann. Meet. Soc. Expl. Geophys., Las Vegas, Nevada, USA, 4-7 June, 2012.

Cordua, K.S., T.M. Hansen, K. Lange, J. Frydendall, and K. Mosegaard, 2012: **"Improving multiple-point-based a priori models for inverse problems by combining Sequential Simulation with the Frequency Matching Method"** (Oral presentation), 82th Ann. Meet. Soc. Expl. Geophys., Las Vegas, Nevada, USA, 4-7 June, 2012.

### Workshop on the State-of-the-Art in Scientific and Parallel Computing (PARA 2012), Helsinki, Finland, 10-13 June, 2012.

Jørgensen, J.B.; Boiroux, D.; Hovgaard, T.G.; Halvgaard, R.; Skajaa, A.; Gade-Nielsen, N.F.; Standardi, L.; Sokoler, L.E.; Völcker, C.; Capolei, A.; Frison, G.; Schmidt, S.; Duun-Henriksen, A.K. 2012: **"Computational Methods for Model Predictive Contro"** (2D/3D (psysical products) - 2D/3D (psysical products)), Workshop on the State-of-the-Art in Scientific and Parallel Computing (PARA 2012), Helsinki, Finland, 10-13 June, 2012

### GERG (European Gas Research Group) Academic Network Event 2012, Brussels, Belgium, 14-15 June 2012

Karakatsani, E.; Kontogeorgis, G.M. 2012: **"Towards the modeling of natural gas systems containing water and selected chemicals"** (Oral presentation), GERG (European Gas Research Group) Academic Network Event 2012, Brussels, Belgium, 14-15 June 2012. Book of presentations

### ANQUE's International Congress of Chemical Engineering (ANQUE-ICCE 2012), 24-27 June 2012, Sevilla, Spain.

Mattei, M.; Kontogeorgis, G.M.; Gani, R. 2012: "Property Prediction for Emulsion Based Chemical Product Design" (Poster presentation), ANQUE's International Congress of Chemical Engineering (ANQUE-ICCE 2012), Sevilla, Spain, 24-27 June, 2012

### 46th US Rock Mechanics/Geomechanics Symposium, Chicago, USA, 24-26 June 2012.

Alam, M. M. ; Fabricius, I. L. ; Hjuler, M.L. ; Christensen, H.F., 2012: "Influence of effective stress coefficient on mechanical failure of chalk". (Oral presentation), 46th US Rock Mechanics / Geomechanics Symposium, Chicago, USA, 24-27 June 2012. Arma 12-286, 10 pp.
Alam, M. M.; Fabricius, I. L., 2012: "Effective stress coefficient for uniaxial strain condition". (Oral presentation), 46th US Rock Mechanics / Geomechanics Symposium, Chicago, USA, 24-26 June, 2012. ARMA 12-302, 6 pp.

### 18th symposium on Thermophysical Properties, Boulder, CO, USA. 24-29 June, 2012.

Mustaffa, A.A.; Kontogeorgis, G.; Kang, J.W.; Gani, R. 2012: "Development and Analysis of Original UNIFAC-CI and Modified UNIFAC-CI Models for Prediction of VLE and SLE Systems" (Poster presentation), 18th symposium on Thermophysical Properties, Boulder, CO, USA. 24-29 June, 2012.

Fosbøl, P.; Thomsen, K. 2012: **"Measurement and modeling of piperazine potassium carbonate solutions for $CO_2$ capture"** (Oral presentation), Eighteenth Symposium on Thermophysical Properties, Colorado, USA, 24-29 June, 2012. Presentation can be found at http://www.staff.dtu.dk/kajt/Presentations

Maribo-Mogensen, B., Kontogeorgis, G. M., Thomsen, K., 2012: **"Comparison of Debye-Hückel and the Mean**

**Spherical Approximation for Electrolyte Equations of State"** (Oral presentation), Eighteenth Symposium on Thermophysical Properties, Colorado, USA, 24-29 June 2012.

Maribo-Mogensen, B., Kontogeorgis, G. M., Tsivintzelis, I., Riaz, M., Michelsen, M., Stenby, E., 2012: **"Recent Applications of the CPA Equation of State for the Petroleum and Chemical Industries"** (Oral presentation), Eighteenth Symposium on Thermophysical Properties, Colorado, USA, 24-29 June 2012.

Thomsen, K. 2012: **"The data bank for electrolyte solutions at CERE DTU Chemical Engineering"** (Poster presentation), Eighteenth Symposium on Thermophysical Properties, Colorado, USA, 24-29 June 2012

Thomsen, K. 2012: **"Recovery of phosphorus for recycling"** (Oral presentation), Eighteenth Symposium on Thermophysical Properties, Colorado, USA, 24-29 June 2012. Presentation can be found at http://www.staff.dtu.dk/kajt/Presentations

### American Control Conference (ACC 2012), Montréal, Canada, 27-29 June 2012.

Capolei, A.; Jørgensen, J.B. 2012: **"Solution of Constrained Optimal Control Problems Using Multiple Shooting and ESDIRK Methods"** (Oral presentation), American Control Conference (ACC 2012), Montréal, Canada, 27-29 June, 2012. Proceedings of the 2012 American Control Conference (ISBN: 978-1-4577-1094-0), 2012.


### ICCR Heriot Watt/ University of Edinburg, Scotland, 2 July, 2012

Fabricius, I. 2012: "Biot´s Coefficeint: A Basic Parameter for Sedimentary Rocks", (Invited Oral Presentation), ICCR Heriot Watt/University of Edinburg, Scotland, 2 July, 2012

### 8th IFAC Symposium on Advanced Control of Chemical Processes, Singapore, 10-13 July 2012.

Zhou, G.; Jørgensen, J.B.; Duwig, C.; Huusom, J.K. 2012: "State Estimation in the Automotive SCR DeNOx Process" (Oral presentation), 8th IFAC Symposium on Advanced Control of Chemical Processes, Singapore, 10-13 July, 2012. Proceedings of 8th IFAC Symposium on Advanced Control of Chemical Processes (ISBN: 9783902823052), pages: 501-506, 2012, DOI: 10.3182/20120710-4-SG-2026.00133

### 11th International Symposium on Process Systems Engineering, Singapore, 15-19 July 2012

Mattei, M.; Kontogeorgis, G.M.; Gani, R. 2012: **"A Systematic Methodology or Design of Emulsion Based Chemical Products"** (Oral highlight presentation + Poster presentation), 11th International Symposium on Process Systems Engineering, 15-19 July 2012, Singapore. Published in the conference proceedings and to be published in Web of Science.

Samad N.A.F.A., Meisler K.T., Gernaey K.V., von Solms N., Gani R. 2012: **"Systematic Identification of Crystallization Kinetics within a Generic Modelling Framework"** (Oral presentation), 11th International Symposium on Process Systems Engineering, Singapore, 15-19 July, 2012. Proceedings of the 11th International Symposium on Process Systems Engineering ed./I.A. Karimi; Rajagopalan Srinivasan. Elsevier BV, 2012 945-949 (Computer Aided Chemical Engineering, 31, 2012)

### 15th International Symposium on Solubility Phenomena and Related Equilibrium Processes, Qinghai, China, 23-27 July, 2012.

Thomsen, K. 2012: **"Thermodynamic modeling of the solubility of alkali and earth alkali borates"** (Oral presentation), 15th International Symposium on Solubility Phenomena and Related Equilibrium Processes, Qinghai, China, 23-27 July, 2012. Presentation can be found at http://www.staff.dtu.dk/kajt/Presentations


### 4th IFAC Nonlinear Model Predictive Control Conference, Noordwijkerhout, The Netherlands, 23-27 August 2012

Hovgaard, T.G.; Larsen, L.F.S.; Jørgensen, J.B.; Boyd, S. 2012: **"Fast Nonconvex Model Predictive** Control for Commercial Refrigeration" (Oral presentation), 4th IFAC Nonlinear Model Predictive Control Conference (NMPC), Noordwijkerhout, The Netherlands, 23-27 August 2012. Proceedings from Nonlinear Model Predictive Control Conference (ISBN: 978-3-902823-07-6), pages: 514-521, 2012, DOI: 10.3182/20120823-5-NL-3013.00082

### 8th IFAC Symposium on Biological and Medical Systems, Budapest, Hungary, 29-31 August 2012.

Boiroux, D.; Duun-Henriksen, A.K.; Schmidt, S.; Nørgaard, K.; Madsbad, S.; Skyggebjerg, O.; Jensen, P.R.; Poulsen, N.K.; Madsen, H.; Jørgensen, J.B. 2012: **"Overnight Control**

**of Blood Glucose in People with Type 1 Diabetes" (**Oral presentation), 8th IFAC Symposium on Biological and Medical Systems, Budapest, Hungary, 29-31 August, 2012. Proceedings of the 8th IFAC Symposium on Biological and Medical Systems, 2012.

Duun-Henriksen, A.K.; Boiroux, D.; Schmidt, S.; Skyggebjerg, O.; Madsbad, S.; Jensen, P.R.; Jørgensen, J.B.; Poulsen, N.K.; Nørgaard, K.; Madsen, H. 2012: **"Tuning of Controller for Type 1 Diabetes Treatment with Stochastic Differential Equations"** (Oral presentation), 8th IFAC Symposium on Biological and Medical Systems, Budapest, Hungary, 29-31 August, 2012. Proceedings of the 8th IFAC Symposium on Biological and Medical Systems, 2012.

### 33rd. IEA EOR Symposium, Regina, Canada, 26-30 August 2012.

Khusainova, A.; Shapiro, A.A.; Stenby, E.H.; Woodley, J.M. 2012: **"Wettability improvement with enzymes: Application to enhanced oil recovery under conditions of the North Sea reservoirs"** (Oral presentation), 33rd. IEA EOR Symposium, Regina, Canada, 26-30 August, 2012. Published in the conference proceedings


### ICAP Technical Meeting, Paris, France, 5-6 September 2012.

Arshad, M.W.; Solms, N. von.: Thomsen, K.; Svendsen, H.F. 2012: "Experimental measurements of heat of absorption of $CO_2$ in DEEA and MAPA" (Oral presentation), ICAP Technical Meeting (EU 7th FP, Cr. No. 241393), Paris, France, 5-6 September 2012

### 13th European Conference on the Mathematics of Oil Recovery (ECMOR XIII), Biarritz, France, 10-13 September 2012.

Capolei, A.; Stenby, E.H.; Jørgensen, J.B. 2012: "High Order Adjoint Derivatives using ESDIRK Methods for Oil Reservoir Production Optimization" (Oral presentation), 13th European Conference on the Mathematics of Oil Recovery (ECMOR XIII), Biarritz, 10-13 September, 2012. Proceedings from ECMOR XIII - 13th European Conference on the Mathematics of Oil Recovery, pages: A42, 2012.

### International Association of Sedimentologists, 29 IAS Meeting of Sedimentologists, Schladming Dachstein, Copenhagen, Denmark, 10-13 September, 2012

Fabricius, I. L., 2012: **"Chalk as a reservoir"**: (Oral presentation), 29th IAS Meeting of Sedimentologists, SchladmigDachstein, Copenhagen, Denmark, 10th-13th September 2012. 1p.

### Advanced Water Management for Oil & Gas Operations, London, UK, 17-19 September 2012.

Karakatsani, E.; Kontogeorgis, G.M. 2012: **"Thermodynamic modelling of natural gas systems containing water and selected chemicals"** (Oral presentation), Advanced Water Management for Oil & Gas Operations, London, UK, 17-19 September 2012.

### GeoENV 2012, Valencia, Spain, 19-21 September, 2012.

Hansen, T.M.; Cordua K.S.; Mosegaard, K. 2012: **"The role of geostatistics as prior information for solving inverse problems"** (Oral presentation), GeoENV 2012, Valencia, Spain, 19-21 September, 2012. Proceedings from GeoENV 2012 can be found at http://geoenv2012.upv.es Symposium 2012, Doha, Qatar, 5-7 March 2012. Printed in conference proceedings

### SPE Applied Technology Workshop on Heavy Oil, Xi´an, China, 23-26 September, 2012

Yan, W. 2012 **"Experimental Methods for Heavy Oil Characterization"** (Oral presentation), SPE Applied Technology Workshop on Heavy Oil, Xi´an, China, 23-26 September, 2012

Yan, W. 2012 **"Prediction of Asphaltene Precipitation - Possibility and Challenge",** (Oral presentation), SPE Applied Technology Workshop on Heavy Oil, Xi´an, China, 23-26 September, 2012


### IEEE International Conference on Control Applications (CCA 2012), Dubrovnik, Croatia, 3-5 October 2012.

Hovgaard, Tobias Gybel ; Larsen, Lars F. S. ; Skovrup, Morten Juel ; Jørgensen, John Bagterp, 2012: **"Analyzing Control Challenges for Thermal Energy Storage in Foodstuffs"** (Oral presentation), IEEE International Conference on Control Applications (CCA 2012), Dubrovnik, Croatia, October 3-5, 2012. Proceedings from 2012 IEEE International Conference on Control Applications (CCA), pages: 956-961, 2012, IEEE

### 26th European Symposium on Applied Thermodynamics, (ESAT), Potsdam, Germany, 7-10 October 2012.

Frost, M.; Solms, N. von; Stenby, E.H.; Kontogeorgis, G.M. 2012: **"Measurements and modeling of phase equilibrium of systems containing polar chemicals"** (Poster presentation), 26th European Symposium on Applied Thermodynamics, (ESAT), Potsdam, Germany, 7-10 October, 2012

Tsivintzelis, I.; Kontogeorgis, G.M. 2012: **"Advanced equations of state for modeling the phase behavior of systems with supercritical, liquid or gaseous $CO_2$"** (Oral presentation), 26th European Symposium on Applied Thermodynamics, (ESAT), Potsdam, Germany, 7-10 October, 2012. Conference Proceedings, Electronic Edition, 26th European Symposium on Applied Thermodynamic, Potsdam, Germany, 7-10/102012

Kontogeorgis, G.M.; Tsivintzelis, I.; Maribo-Mogensen, B. 2012 **"Association theories - what is possible, what is difficult, what is new"** (Oral presentation), 26th European Symposium on Applied Thermodynamics, (ESAT), Potsdam, Germany, 7-10 October, 2012. Abstract in Conference Proceedings, Electronic Edition, 26th European Symposium on Applied Thermodynamic, Potsdam, Germany, 7-10/102012

Liang, X.; Kontogeorgis, G.M. 2012: **"What can we learn from putting speed of sound data into the universal constants regression in PC-SAFT"** (Poster presentation), 26th European Symposium on Applied Thermodynamics, (ESAT), Potsdam, Germany, 7-10 October, 2012

Maia, F.M.; Tsivintzelis, I.; Rodriques, O.; Macedo, E.A.; Kontogeorgis, G.M. 2012: **"The CPA equation of state applied to systems with ionic liquids"** (Oral presentation), 26th European Symposium on Applied Thermodynamics, (ESAT), Potsdam, Germany, 7-10 October, 2012. Abstract in Conference Proceedings, Electronic Edition, 26th European Symposium on Applied Thermodynamic, Potsdam, Germany, 7-10/102012

### Equifase 2012, Puerto Varas, Chile 8-12 October 2012.

Michelsen, M.L. 2012: **"Computational methods: Status and perspectives"**, (Invited lecture), Equifase 2012, Puerto Varas, Chile, 8-12 October, 2012

### 2012 American Institute of Chemical Engineering Annual Meeting, Pittsburgh, USA, 28 October-2 November, 2012

Mattei, M.; Hill, M.; Kontogeorgis, G.M.; Gani, R. 2012: **"Design of an Emulsified Hand Wash through a Systematic Model-based Methodology"** (Oral presentation), 2012 American Institute of Chemical Engineering Annual Meeting, 28 October-2 November 2012, Pittsburgh, USA. Abstract published in the conference proceedings.

Meisler K.T., Samad, N.A.F.A., von Solms N., Gernaey K.V. and Gani R. 2012: **"Crystallization Kinetics Identification within a Generic Modeling"** (Oral presentation), 2012 AIChE Annual Meeting, Pittsburgh, USA, 28 October-2 November 2012.

Karakatsani, E.; Kontogeorgis, G.M. 2012: **"Calculating Dew Points for Natural Gas Containing Water and/or Selected Production Chemicals"** (Oral presentation), 2012 AIChE Annual Meeting, Pittsburgh, USA, 28 October-2 November 2012.


### EAGE 2012, Copenhagen, Denmark, 5-9 November, 2012.

Cordua, K.S., T.M. Hansen, and K. Mosegaard, 2012: "Monte Carlo based tomographic full waveform inversion with multiple-point a priori information" (Oral presentation), EAGE 2012, Copenhagen, Denmark, 5-9 November, 2012.

### 10th European Workshop on Advanced Control and Diagnosis, Lyngby, Denmark, 8-9 November, 2012.

Olesen, D.H.; Huusom, J.K.; Jørgensen, J.B. 2012: **"Optimization based tuning approach for offset free MPC"** (Oral presentation), 10th European Workshop on Advanced Control and Diagnosis, Lyngby, Denmark, 8-9 November, 2012. Proceedings from The 10th European Workshop on Advanced Control and Diagnosis, 2012.

Sokoler, L.E.; Edlund, K.; Frison, G.; Skajaa, A.; Jørgensen, J.B. 2012: **"Real-Time Optimization for Economic Model Predictive Control"** (Oral presentation), 10th European Workshop on Advanced Control and Diagnosis, Lyngby, Denmark, 8-9 November, 2012. Proceedings from The 10th European Workshop on Advanced Control and Diagnosis (ACD 2012), 2012.

Standardi, L.; Edlund, K.; Poulsen, Kjølstad, N.; Jørgensen, J.B. 2012: **"A Dantzig-Wolfe Decomposition Algorithm**

**for Linear Economic MPC of a Power Plant Portfolio"** (Oral presentation), 10th European Workshop on Advanced Control and Diagnosis, Lyngby, Denmark, 8-9 November, 2012. Proceedings from The 10th European Workshop on Advanced Control and Diagnosis (ACD 2012), 2012.

Gade-Nielsen, N.F.; Jørgensen, J.B.; Dammann, B. 2012: **"MPC Toolbox with GPU Accelerated Optimization Algorithms"** (Oral presentation), 10th European Workshop on Advanced Control and Diagnosis, Lyngby, Denmark, 8-9 November, 2012. Proceedings from The 10th European Workshop on Advanced Control and Diagnosis (ACD 2012), 2012.

Hovgaard, T.G.; Larsen, L.F.S.; Jørgensen, J.B. 2012: **"Sequential Convex Programming for Power Set-point Optimization in a Wind Farm using Black-box Models, Simple Turbine Interactions, and Integer Variables"** (Oral presentation), 10th European Workshop on Advanced Control and Diagnosis, Lyngby, Denmark, 8-9 November, 2012. Proceeding of the 10th European Workshop on Advanced Control and Diagnosis, 2012.

### EAGE 2012, Copenhagen, Denmark, 5-9 November, 2012

Cordua, K.S., T.M. Hansen, and K. Mosegaard, 2012: **"Monte Carlo based tomographic full waveform inversion with multiple-point a priori information"** (Oral presentation), EAGE 2012, Copenhagen, Denmark, 5-9 November, 2012.

### 11th International Conference of Greenhouse Gas Control Technologies (GHGT-11), Kyoto, Japan, 18-22 November 2012.

Arshad, M.W.; Solms, N. von.: Thomsen, K.; Svendsen, H.F. 2012: "Heat of absorption of $CO_2$ in aqueous solutions of DEEA, MAPA and their mixture" (Poster presentation), 11th International Conference of Greenhouse Gas Control Technologies (GHGT-11), Kyoto, Japan, 18-22 November, 2012. To be published in Energy Procedia

Fosbøl, P.; Maribo-Mogensen, B.; Thomsen, K. 2012: **"Solids Modelling and Capture Simulation of Piperazine in Potassium Solvents"** (Oral presentation), 11th International Conference of Greenhouse Gas Control Technologies (GHGT-11), Kyoto, Japan, 18-22 November, 2012.

Valenti, G.; Bonalumi, D.; Macchi, E.; Gatti, D.; Fosbøl, P.; Thomsen, K. 2012: **"Alternative Layouts for the Carbon Capture with the Chilled Ammonia Process"** (Oral presentation), 11th International Conference of Greenhouse Gas Control Technologies (GHGT-11), Kyoto, Japan, 18-22 November, 2012.

### EAGE conference "Integrated reservoir modelling. Dubai, 25-28 November 2012.

Melnikova Y., Cordua K.S., Mosegaard K. 2012: **"History matching: towards geologically reasonable models" (Oral presentation), EAGE conference "Integrated reservoir modelling. Are we doing it right?"**, Dubai, 25-28 November, 2012. Proceedings from EAGE conference "Integrated reservoir modelling. Are we doing it right?", 2012.


### GEUS, Copenhagen, Denmark, 11 December, 2012

Rosenbrand, E. 2012: "Fines Migration in Sandstone: Remarkably Well Predicted by the DLVO Theory", (Invited Oral presentation), GEUS, Copenhagen, Denmark, 11 December, 2012

### ICCR-SCTC, Workshop, Rio de Janeiro, Brazil, 12 December, 2012

Fabricius, I. 2012: "The Diagenetic Front", (Invited Oral presentation), ICCR-SCTC, Workshop, Rio de Janeiro, Brazil, 12 December, 2012.

# Master Thesis 2012

**Megbal Aissa**
Measurement and modeling of $CO_2$ absorption in amino acid salt solutions

**Sofie Holme Bartholdy**
Modeling of adsorption equilibrium on molecular sieves and silica gels by AST and Langmuir

**Martin Gamel Bjørner**
Modeling of adsorption on molecular sieves and silica gel using the Potential Adsorption Theory

**Kristian Hedberg Eisenhardt**
Amino acid salt solutions for $CO_2$ capture

**Daniel Kunish Eriksen**
Towards the development of a polar CPA equation of state

**Søren Skov Hansen**
Numerical methods for simulation and optimization of oil production

**Asger Johansen**
AVO analysis and rock physics based AVO inversion - Predicting hydrocarbons and the properties of North Sea greensand

**Adam Samir Kadhim**
Optimization of industrial crystallization process

**Turgay Kart**
Optimization of industrial crystallization process

**Thomas Christian Krüger**
Modeling the conductivity of salt solutions

**Dariusz Michal Lerch**
Modelling and Production Optimisation of Oil Reservoirs.

**Henrik Lund Nielsen**
Design, simulation, and energy optimization of $CO_2$ reduction process

**Jacob Fabricius Riis**
Shallow fresh water in central North Sea

**Irene Gallo Stampine, Erasmu**s
Solidification of Amino Acids in CO2 Capture
Dariusz Lerch
Modelling and Production Optimisation of Oil Reservoirs

**Søren Skov Hansen**
Numerical Methods for Simulation and Optimization of Oil Production

**Daniel H. Olesen**
Tuning Methods for Model Predictive Controllers

**Gianluca Frison**
Numerical Methods for Model Predictive Control

**Leo Emil Sokoler**
Second-Order Cone Programming for Probabilistic MPC in Power Production Management

**Morten Steen Nielsen & Daniel Witt Johansen**
Model Predictive Control and Simulation of a Biochemical Process in a U-Loop Reactor

**Franck Engoulevent**
Simulation, Control and Optimization of Single-Cell Protein Production in a U-Loop Reactor

**Guofeng Zhou** [co-supervisor - together with Jakob K. Huusom from CAPEC]
Model Based Control and Monitoring of the SCR Process for Diesel Engines

# Publications 2012

**Previously submitted manuscripts, published in 2012**

**CERE 1029** "Comparing Ignitability for In Situ Burning of Oil Spills for an Asphaltenic, a Waxy and a Light Crude Oil as a Function of Weathering Conditions under Arctic Conditions". **J. Fritt-Rasmussen, P.J. Brandvik, A. Villumsen, and E.H. Stenby.** Cold Region Science and Technology, 72 (2012) 1-6)

**CERE 1046** "Monte Carlo Full Waveform Inversion of Crosshole GPR Data using Multiple-point Geostatistical a Priori Information". **Knud S. Cordua, Thomas M. Hansen, and Klaus Mosegaard.** (Geophysics, 77(2) (2012) H19-H-31)

**CERE 1102** "Novel Self-Associative and Multiphase Nanostructured Soft Carriers based on Amphiphilic Hyaluronic Acid Derivatives" **Corinne Eenschooten, Andrea Vaccoro, Florence Delie, Fanny Guillaumie, Kristoffer Tømmeraas, Georgios M. Kontogeorgis, Khadija Schwach-Abdellaoui, Michal Borkovec, and Robert Gurny** (Carbohydrate Polymers, 87(1) (2012) 444-451)

**CERE 1113** "Vp-Vs Relationship and Amplitude Variation with Offset Modelling of Glauconitic Greensand" **Z. Hossain, T. Mukerji, and I.L. Fabricius** (Geophysical Prospecting, 60 (2012) 117-137)

**CERE 1115** "Application of sPC-SAFT to glycol ethers". **Ane S. Avlund, Georgios M. Kontogeorgis, and Michael L. Michelsen.** (Industrial & Engineering Chemistry Research, 51(1) (2012) 547-555)

**CERE 1118** "Experimental Study and Phase Equilibrium Modeling of Systems Containing Acid Gas and Glycol". **Waheed Afzal, Martin P. Breil, Ioannis Tsivintzelis, Amir H. Mohammadi, Georgios M. Kontogeorgis, and Dominique Richon.** (Fluid Phase Equlibria, 318 (2012) 40-50)

**CERE 1120** "Thermodynamically based Solvent Design for Enzymatic Saccharide Acylation with Hydroxycinnamates in Non-conventional Media. **Birgitte Zeuner, Georgios M. Kontogeorgis, Anders Riisager, and Anne S. Meyer.** (New Biotechnology, 29(3) (2012) 255-270)

**CERE 1121** "30 Years with EoS/GE Models - what have we learnt?". **Georgios M. Kontogeorgis, and Philippos Coutsikos.** (Industiral & Engineering Chemistry Research, 51(11) (2012) 4119-4142)

**CERE 1123** "Gravity Effect on Two-Phase Immiscible Flows in Communicating Layered Reservoirs". **Xuan Zhang, Alexander Shapiro, and Erling H. Stenby.** (Transport in Porous Media, 92 (2012) 767-788)

**CERE 1126** "Selective oxidation of benzyl alcohol in dense $CO_2$: insight by phase behavior modeling". **Matthias Josef Beier, Jan-Dierk Grunwaldt, Ioannis Tsivintzelis, Anker D. Jensen, Georgios M. Kontogeorgis, and Alfons Baiker.** (Journal of Supercritical Fluids, 63 (2012) 199-207)

**CERE 1128** "Phase Equilibria of Three Binary Mixtures; Methyl mercaptan + Methane, Methyl mercaptan + Nitrogen and Methyl mercaptan + Carbon dioxide; Experimental data & Modeling". J**aveed Awan, Ioannis Tsivintzelis, Christophe Coquelet, and Georgios M. Kontogeorgis.** (Journal of Chemical & Engineering Data, 57 (2012) 896-901)

**CERE 1130** "Colloid Transport and Retention: Recent Advances in Colloids Filtration Theory" **Hao Yuan, and Alexander A. Shapiro** (Chapter for the book "Colloids: Classification, Properties and Applications", Nova Science Publishers, NY, USA, 2012)

**CERE 1137** "Comparison of the Debye-Hückel and the Mean Spherical Approximation Theories for Electrolyte Solutions". **Bjørn Maribo-Mogensen, Georgios M. Kontogeorgis, and Kaj Thomsen.** (Industrial and Engineering Chemistry Research, 51 (2012) 5353-5363)

**CERE 1138** "Limits to Nonlinear Inversion. In: Kristján Jónasson (ed.)" **K. Mosegaard** (Applied Parallel and Scientific Computing, 10th International Conference, PARA 2110, Reykjavik, Iceland, June 6-9, 2010: Revised Selected Papers, Part 1. Springer, 2012 11-21 (Lecture Notes in Computer Science; No. Part 1, Vol 7133)

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**New manuscripts in 2012**

**CERE 1201** "A New Comprehensive Approach for Predicting Injectivity Decline during Waterflooding". **H. Yuan, S. M. Nielsen, and A. A. Shapiro.** (SPE 154509, 2012)

**CERE 1202** "A Systematic Methodology for Design of Emulsion Based Chemical Products" **Michele Mattei, Georgios M. Kontogeorgis, and Rafiqul Gani**

(Proceedings of the 11th International Symposium on Process Systems Engineering. 15-19 July 2012, Singapore Ed./I.A. Karimi; rajagopalan Srinivasan. Elsevier BV, Computer Aided Chemical Engineering 31 (2012) 220-224)

**CERE 1203** "Equation of State Modelling of Systems with Ionic Liquids: Literature Review and Application with the Cubic Plus Association (CPA) model" **Filipa M. Maia, Ioannis Tsivintzelis, Oscar Rodriguez, Eugénia A. Macedo, Georgios M. Kontogeorgis** (Fluid Phase Equilibria, 332 (2012) 128-143)

**CERE 1204** "Vapor-Liquid-Liquid-Equilibrium Measurements and Modeling of the Methanethiol + Methane + Water ternary System at 304, 334 and 364 K". **Javeed A. Awan, Ioannis Tsivintzelis, Alain Valtz, Christophe Coquelet, and Georgios M. Kontogeorgis.** Industrial and Engineering Chemistry Research, 51 (2012) 11561-11564

**CERE 1205** "Kinetics of Absorption of Carbon Dioxide into Aqueous Potassium Salt of Proline". **Subham Paul, and Kaj Thomsen.** (International Journal of Greenhouse Gas Control, 8 (2012) 169-179)

**CERE 1206** "Comparison of Two Electrolyte Models for the Carbon Capture with Aqueous Ammonia" .**Victor Darde, Kaj Thomsen, Willy J.M. van Well, Davide Bonalumi, Gianluca Valenti, and Ennio Macchi.** (International Journal of Greenhouse Gas Control, 8 (2012) 61-72)

**CERE 1207** "Phase Equilibrium modeling of gas hydrate systems for $CO_2$ Capture". **Peter Jørgensen Herslund, Kaj Thomsen, Jens Abildskov, and Nicolas von Solms.** (Journal of Chemical Thermodynamics, 48 (2012) 13-27)

**CERE 1209** "Static and Dynamic Effective Stress Coefficient of Chalk". **M.M. Alam, I.L. Fabricius, and H.F. Christensen.** (Geophysics, 77(2) (2012) L1-L11)

**CERE 1210** "Thermally Induced Permeability Reduction due to Particle Migration in Sandstones: The effect of Temperature on Kaolinite Mobilisation and Aggregation". **R. Rosenbrand, I.L. Fabricius and H. Yuan.** (Thirty-Seventh Workshop on Geothermal Reservoir Engineering, Standford University, Stanford, California, January 30 – February 1, 2012 SGP-TR-194)

**CERE 1211** "A Frequency Matching Method for Generation of a Priori Sample Models from Training Images". **Katrine Lange, Knud Skou Cordua, Jan Frydendall, Thomas Mejer Hansen, and Klaus Mosegaard.** (Proceedings from Annual Conference of the International Association for Mathematical Geosciences, IAMG 2011, Salzburg, Austria)

**CERE 1212** "Transport Properties of Natural Gas through Polyethylene Nanocomposites at High Temperature and Pressure". **Jimoh K. Adewole, Lars Jensen, Usamah A. Al-Mubaiyedh, Nicolas von Solms, and Ibnelwaleed A. Hussein.** (J. Polm. Res. 19, 9814 (2012)

**CERE 1213** "A New Pilot Absorber for $CO_2$ Capture from Flue Gases: Measuring and Modelling Capture with MEA Solution" **Tim L. Sønderby, Kim B. Carlsen, Philip L. Fosbøl, Lars G. Kiørboe, and Nicolas von Solms** (International Journal of Greenhouse Gas Control, 12 (2013) 181-192)

**CERE 1214** "Mechanisms of Advanced Waterflooding in Chalk Reservoirs: Role of Seawater-Crude Oil Interactions". **Sara Bülow Sandersen, Adeel Zahid, Erling H. Stenby, Nicolas von Solms, and Alexander Shapiro.** (Submitted to Journal of Colloids and Surfaces A: Physicochemical and Engineering Aspects)

**CERE 1215** "The Effect of Pressure on the Phase Behavior of Surfactant Systems: An Experimental Study" **Sara Bülow Sandersen, Erling H. Stenby, and Nicolas von Solms** (Colloids and Surfaces A: Physicochemical and Engineering Aspects, 415 (2012) 159-166)

**CERE 1216** "Reaction Kinetics for the Desorption of $CO_2$ from Aqueous MEA – Experiments and Modelling". **Niels V. Bagger, Peter Lützen, Lars G. Kiørboe, and Nicolas von Solms.** (Submitted to International Journal of Greenhouse Gas Control)

**CERE 1217** "Development and Testing of a New Apparatus for the Measurement of High-Pressure Low-Temperature Phase Equilibria" **José M. Fonseca, and Nicolas von Solms** (Fluid Phase Equilibria, 329 (2012) 55-62)

**CERE 1218** "Modeling Solubility and Swelling in Supercritical Carbon Dioxide – Polymer Systems". **Rasmus Lundsgaard, Christian Wang, Adam Rubin, and Nicolas von Solms.** (Internal Report)

**CERE 1219** "Calculation of Minimum Miscibility Pressure using Fast Slimtube Simulation". **W. Yan, M.L. Michelsen, and E.H. Stenby.** (SPE 153758 – presented at the 18th SPE Improved Oil Recovery Symposium held in Tulsa, Oklahoma, USA, April, 2012)

**CERE 1220** "A Comparative Study of Reduced Variables Based Flash and Conventional Flash" **M.L.**

**Michelsen, W. Yan, and E.H. Stenby** (SPE 154477 – presented at the EAGE Annual Conference and Exhibition incorporating SPE Europec, Copenhagen, Denmark, June 2012)

**CERE 1221** "On Multiphase Negative Flash for Ideal Solutions". **W. Yan, and E.H. Stenby.** (Fluid Phase Equilibria, 322-323 (2012) 41-47)

**CERE 1222** "On Application of Non-cubic EoS to Compositional Reservoir Simulation". **W. Yan, M.L. Michelsen, and E.H. Stenby.** (SPE 142995 – presented at the SPE EUROPEC/EAGE Annual Conference and Exhibition, Vienna, Austria, May, 2011)

**CERE 1223** "Comparison of Two Methods for Speeding Up Flash Calculations in Compositional Simulations".
**A. Belkadi, W. Yan, M.L. Michelsen, and E.H. Stenby.** (SPE 142132 – presented at the SPE Reservoir Simulation Symposium, The Woodlands, Texas, USA, February, 2011)

**CERE 1225** "Fluid Phase Equilibira of the Reaction Mixture during the Selective Hydrogeneration of 2-butanal in Dense Carbon Dioxide" **Nikolai E. Musko, Anker Degn Jensen, Alfons Baiker, Georgios M. Kontogeorgis, and Jan-Dierk Grunwaldt** (Applied Catalysis A: General, 443-444 (2012) 67-75)

**CERE 1226** "Fluid Phase Equilibria during Propylene Carbonate Synthesis from Propylene Oxide in Carbon Dioxide Medium". **Loubna Gharnarti, Nikolai E. Musko, Anker Degn Jensen, Georgios M. Kontogeorgis, and Jan-Dierk Grunwaldt.** (Submitted for publication)

**CERE 1227** "Managing Injected Water Composition To Improve Oil Recovery: A Case Study of North Sea Chalk Reservoirs". **Adeel Zahid, Alexander Shapiro, Erling H. Stenby, and Wei Yan.** (Enery Fuels, 26 (2012) 3407-3415)

**CERE 1228** "Estimating Filtration Coefficients for Straining from Percolation and Random Walk Theories"
**Hao Yuan, Alexander Shapiro, Zhenjiang You, and Alexander Badalyan** (Chemical Engineering Journal, 210 (2012) 63-73)

**CERE 1229** "Approach to Improve Speed of Sound Calculation within PC-SAFT Framework" **Xiaodong Liang, Bjørn Maribo-Mogensen, Kaj Thomsen, Wei Yan, and Georgios M. Kontogeorgis** (Industrial and Engineering Chemistry Research, 51(45) (2012) 14903-14914)

**CERE 1231** "Wettability Improvement with Enzymes: Application to Enhanced Oil Recovery under Conditions of the North Sea Reservoirs". **Alsu Khusainova, Alexander A. Shapiro, Erling H. Stenby, and John M. Woodley.** (Presentation for the 33rd. IEA EOR Symposium, Saskatchewar, Canada, August 26-30, 2012)

**CERE 1232** "Capabilities and Limitations of an Association Theory for Chemicals" **Ioannis Tsivintzelis, and Georgios M. Kontogeorgis** (Industrial & Engineering Chemistry Research, 51(41) (2012) 13496-13517)

**CERE 1235** "Evaluation and Extension of the GC-PPC-SAFT Equation of State for VLE and LLE of Hydrocarbons and Oxygenated Compounds. Part I". **Thanh-Binh Nguyen, Jean-Charles de Hemptinne, Benoit Creton, and Georgios M. Kontogeorgis.** (Submitted for publication)

**CERE 1236** "The Conversion of Cardiovascular Conference Abstracts to Publications". **Emil L. Fosbøl, Philip L. Fosbøl, Robert A. Harrington, Eapen Zubin, and Eric D. Peterson.** (Circulation, 126(24), (2012) 2819-2825)

**CERE 1237** "Prediction of Thermo-Physical Properties of Liquid Formulated Products". **Michele Mattei, Elisa Conte, Kontogeorgis, and Rafiqul Gani.** Will be published in (Product Design and Engineering, Volume III: Paste and Gel Formulations", edited by Wiley)

**CERE 1238** "Thermodynamic Properties and Models for Engineering Applications". **Georgios M. Kontogeorgis.** (Chemical Engineering and Chemical Process Technology, [Eds. UNESCO-EOLSS Joint Committee], in Encyclopedia of Life Support Systems (EOLSS), Developed under the Auspices of the UNESCO, Eolss Publishers, Oxford, UK)

**CERE 1239** "A Frequency Matching Method: Solving Inverse Problems by Use of Geologically Realistic Prior Information" **Katrine Lange, Jan Frydendall, Knud Skou Cordua, Thomas Mejer Hansen, Yulia Melnikova, and Klaus Mosegaard** (Mathematical Geosciences, 44(7), (2012) 783-803)

**CERE 1240** "Effects of Everyday Life Events on Glucose, Insulin, and Glucagon Dynamics in Continuous Subcutaneous Insulin Infusion – Treated Type 1 Diabetes: Collection of Clinical Data for Glucose Modeling" **Signe Schmidt, Daniel Aaron Finan; Anne Katrine Duun-Henriksen, John Bagterp Jørgensen, Henrik Madsen, Henrik Bengtsson, Jen Juul Holst,**

**Sten Madsbad and Kirsten Nørgaard** (Diabetes Technology & Therapeutics, 14(3), (2012) 210-217)

**CERE 1241** "Model Predictive Control Technologies for Efficient and Flexible Power Consumption in Refrigeration Systems" **Tobias Gybel Hovgaard, Lars F.S. Larsen, Kristian Edlund, and John Bagterp Jørgensen** (Energy, 44(1) (2012) 105-116)

**CERE 1242** "Optimal Energy Consumption in Refrigeration Systems - Modelling and Non-Convex Optimisation" **Tobias Gybel Hovgaard, Lars F.S. Larsen, Morten J. Skovrup, and John Bagterp Jørgensen (**Canadian Journal of Chemical Engineering, 90(6), (2012) 1426-1433)

**CERE 1243** "Tuning SISO Offset-free Model Predictive Control Based on ARX Models" **Jakob Kjøbsted Huusum, Niels Kjølstad Poulsen, Sten Bay Jørgensen, and John Bagterp Jørgensen** (Journal of Process Control, 22(10), (2012) 1997-2007)

CERE 1244 "Fast Nonconvex Model Predictive Control for Commercial Refrigeration" Tobias Gybel Hovgaard, Lars F.S. Larsen, John Bagterp Jørgensen, Stephen Boyd (Nonlinear Model Predictive Control Conference, 4 International Federation of Automatic Control, (2012) 514-521)

**CERE 1245** "Process Simulation of $CO_2$ Capture with Aqueous Ammonia Using the Extended UNIQUAC Model" **Victor Darde, Bjørn Maribo-Mogensen, Willy J.M. van Well, Erling H. Stenby, and Kaj Thomsen** (International journal of Greenhouse Gas Control, 10 (2012) 74-87)

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