

# CERE

ANNUAL  
REPORT 2013

A large, stylized world map composed of numerous small, dark gray dots, set against a black background. The map is centered and occupies most of the lower half of the page.

CENTER FOR ENERGY RESOURCES ENGINEERING





**CERE Annual Report 2013**

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The high level of scientific activity at the center is reflected in numerous conference contributions and publications throughout the year.

# From Daring Blue Sky to Market Implementation



Professor  
Erling H. Stenby,  
Chairman of CERE

Welcome to the CERE Annual Report 2013. We have a lot to tell, both when looking back and forward. The year 2013 has been very productive and prosperous for CERE and I hope you will enjoy reading about some selected highlights in this report.

Today, as from the very beginning more than 30 years ago, CERE covers the entire scale of research. We have projects that seek out new frontiers and strive for improved understanding of fundamental questions; we have projects very close to application; and we have everything in between.

Another trademark is our international bonds. CERE has always been involved in projects with broad applications. This is documented not only by the list of our academic partners abroad, but maybe even more so by the members of our industrial Consortium. All 29 members operate on an international, if not global scale, the vast majority being headquartered outside Denmark.

## The broader scope

In this appetizer for the Annual report 2013, I want to emphasize the dynamic setup in CERE. The composition of our disciplines and the quality of our academic resources enable us to be highly flexible and quickly set up cross-disciplinary collaborations when needed, both for fundamental and more applied projects.

The choice of the network metaphor as the visual underlining of this report is thus not a coincidence. We go across the relevant departments at DTU for the cutting-edge competencies, and we connect, when the interest is there, industrial partners with similar challenges and interests in state-of-the-art projects. Last but not least, we cover the globe with our portfolio of ambitious research programs, ranging from daring blue sky to the very edge of market implementation.

As a new development our good colleague, Professor Klaus Mosegaard, has decided to move to a position at the Niels Bohr Institute at University of Copenhagen as of 1 April 2014.

We wish to continue our excellent collaboration with Klaus and will therefore make sure that this will continue after he leaves DTU. This means that the ongoing and newly started projects will be carried out as planned and you will meet Klaus at the CERE Discussion Meeting in June.

## New important initiative for the Danish Oil sector

In 2013 it was announced that the Danish Underground Consortium (DUC) wishes to establish a national Danish research center for applied oil and gas research, with specific focus on the Danish North Sea. DUC has the following partners: Maersk Oil, Shell, Chevron and Nordsøfonden. The center will be headquartered at DTU and involve research groups at several Danish universities in collaboration with the DUC partners.

I see this as a very positive development for Denmark and the possibilities to exploit our country's energy resources, and I am convinced the new center will provide great opportunities for synergy through collaboration with CERE.

## A ticket for knowledge

In this 2013 issue, we focus on a specific type of projects in the center, i.e. the Joint Industry Projects (JIPs). Here several industrial partners team up to develop a research program. The gain for each participant is vast, since with a limited contribution a company can benefit from the entire pool of results generated by a large project, while adding their specific angle of interest to the scope.

With a reference to our very recent large research grant and JIP from the Danish National Foundation for Advanced Technology (also described within the report), CERE is the OPTION that will create new and promising results in your R&D activities.

We look forward to another exciting year of cross-disciplinary cutting-edge collaborations in 2014, and I hope to see you at the annual CERE Discussion Meeting, 25-27 June 2014.



# Proudly presenting: The Faculty of CERE

What are the fields of special interest to the members of CERE's Faculty? We have asked the people that constitute the academic core of the center to introduce themselves and their research in short videos.

*Optimization of oil recovery and modeling of smart energy systems are trademarks of Associate Professor John Bagterp Jørgensen, DTU Compute.*

*John Bagterp Jørgensen*



*Kinetic inhibition of gas hydrates take up a large proportion of the work time of Associate Professor Nicolas von Solms, DTU Chemical Engineering.*

*Nicolas von Solms*



*Senior Scientist Wei Yan, DTU Chemistry, fills a position of strategic importance to CERE. He engages in both experimental and theoretical thermodynamics.*

*Wei Yan*



*Enhanced Oil Recovery is a topic close to the heart of Professor Erling H. Stenby, DTU Chemistry Director – and Chairman of CERE.*

*Erling H. Stenby*



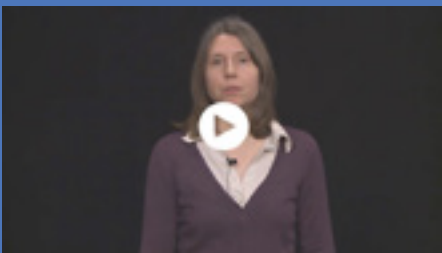
*Integration of rock mechanical, geophysical and geological information is a cornerstone in the work done by Professor Ida Lykke Fabricius, DTU Civil Engineering.*

*Ida Lykke Fabricius*



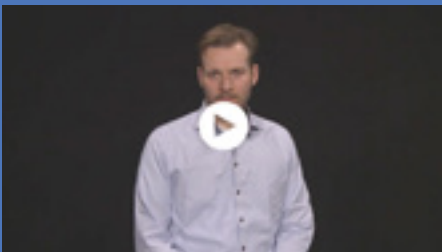
*Mechanical properties of chalk and other types of rock is the main field of interest to Assistant Professor Katrine Alling Andreassen, DTU Civil Engineering.*

*Katrine Alling Andreassen*



*Carbon capture and other CO<sub>2</sub> related issues – i.e. transportation, corrosion – are the main focuses of Assistant Professor Philip L. Fosbøl, DTU Chemical Engineering.*

*Philip L. Fosbøl*



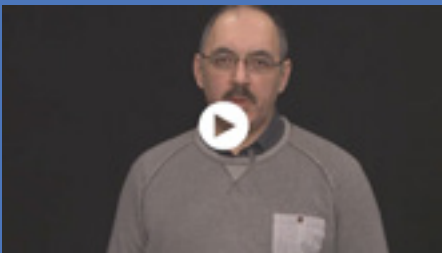
*Thermodynamic modeling of reactions involving electrolytes is just one example of the broad range of topics covered by Associate Professor Kaj Thomsen, DTU Chemical Engineering.*

*Kaj Thomsen*



*Using microorganisms and/or enzymes for enhanced oil recovery is a current area of top focus for Associated Professor Alexander A. Shapiro, DTU Chemical Engineering.*

*Alexander A. Shapiro*





# Simulation of Oil Well Flow becomes an OPTION

“Project OPTION will be central to our ability to improve the prediction of the recovery factor and thereby assist our clients to assess measures that must be implemented to optimize recovery.”

Claus Myllerup, Senior Vice President, Technology, Lloyd's Register Energy.

A new Joint Industry Project combines reservoir modeling, chemical engineering, computational fluid dynamics (CFD), and uncertainty estimates. The ambition is to create a new class of tools for practical use especially for horizontal wells.

Oil production is a dynamic operation in which the various wells are typically interdependent: The rate of production at one well may influence the expected output from another well either positively or negatively. Until now it has been considered too complex for accurate simulations to find the optimal solution for the entire field in question, but a new Danish Joint Industry Project (JIP) has just that ambition.

The OPTION project (Optimizing Oil Production by Novel Technology Integration) integrates several highly different disciplines across DTU and is led by CERE. Professor Erling H. Stenby, Chairman of CERE, is responsible for coordinating the DTU part of the project and represents DTU in the OPTION steering committee. The project is supported by a close to 2.0 million EUR grant from the Danish National Advanced Technology Foundation. Industry partners are Welltec and Lloyd's Register Energy, including Senergy that is now a part of the Lloyds Register Group.

The total budget for OPTION is 4.0 million EUR. The project's perspective is for the increased understanding of the interface between reservoir and well performance to improve well and completion design to enhance productivity and oil recovery. If successful, even a 1% increase in oil recovery from Danish fields would represent an estimated value of approx. 8 billion EUR to the Danish economy.

## Enhancing recovery factors

Various reservoir management regimes have been suggested to maximize oil recovery of a

given reservoir. The control input for can be well rates, bottom-hole pressures, valve/choke settings, and others. Typically, the focus is not at maximizing oil production in absolute terms, but rather at maximizing economic gain measured as the value of the oil produced relative to cost of production. In other words the goal is to maximize the net present value of a given oil reservoir over the entire life time of the reservoir.

*“We are delighted to have been awarded funding from the Danish National Advanced Technology Foundation as the research and techniques within this project will become central for the ability to improve predictions of reservoir recovery rates. Project OPTION will be central to our ability to improve the prediction of the recovery factor and thereby assist our clients to assess measures that must be implemented to optimize recovery. The project will clearly strengthen the expansion of our Danish business in the global market,”* says Claus Myllerup, Senior Vice President Technology at Lloyd's Register Energy.

## Upgrading the process of qualification

Welltec participates in a CERE JIP for the first time. The company develops and provides well technology and solutions for the oil and gas industry. Its technology and solutions are dedicated to aid in optimizing the performance of reservoirs by providing the necessary solutions to do so, both in the form of well completion technology and intervention solutions which ensure the well performance and integrity.

*“This project has the potential for yielding unique insights that may improve our activities within well infrastructure considerably. If, as we expect, the project succeeds, we will be able to upgrade our process of qualification significantly, just as our solutions will gain further in trustworthiness,”* says Welltec CEO Jørgen Hallundbæk.

## Results will surely be put to use

In the OPTION project such reservoir management regimes will be investigated. Further, will skills in reservoir modeling, chemical engineering, and CFD, present at various DTU departments (DTU Chemical Engineering, DTU Space, DTU Chemistry, DTU Civil Engineering, and DTU Mechanics), be integrated. Also, quantification of the in-avoidable uncertainties inherent in the found solutions will form a key element in the project.

*“We are pleased to welcome both Welltec as new CERE JIP participant, just as the projects represents a higher level of cooperation with Lloyd's Register Energy,”* says CERE chairman Erling H. Stenby.

*“The industry involvement guarantees that the results of the project will be put to use, as all three companies have a wide portfolio of clients for consultancy services in the industry. And while OPTION does not have direct users – oil and gas producing companies – as partners just now, we surely imagine this to be possible a bit further down the road.”*

Sources: [www.lr.org](http://www.lr.org) / [www.hoejtekknologifonden.dk](http://www.hoejtekknologifonden.dk)

Danish National Advanced Technology Foundation press release: [http://hoejtekknologifonden.dk/nyheder/nyhedsoversigt/investeringer\\_for\\_583\\_millioner\\_kroner\\_starter\\_nye\\_danske\\_teknologieventyr/matematik\\_skal\\_omsaettes\\_til\\_mereolie/](http://hoejtekknologifonden.dk/nyheder/nyhedsoversigt/investeringer_for_583_millioner_kroner_starter_nye_danske_teknologieventyr/matematik_skal_omsaettes_til_mereolie/)



# Join the JIP's

"...Often it is only the challenge that is obvious and we have to develop the ideas for solutions together. This often forms the basis for PhD projects, design of new equipment, or development of new software."



Erling H. Stenby, Professor, CERE Chairman.

A cornerstone in CERE's activity is the ability to set up robust and ambitious Joint Industry Projects (JIP) quickly and without too much administrative trouble for the partners involved.

The portfolio of Joint Industry Projects at CERE keeps evolving. They present a chance for a company to dwell deeper into a subject of special interest for a period of at least three years.

"By entering a JIP, a company has the advantage of taking part in a major research scheme through a limited commitment. Funding one PhD student or Post Doc plus operational expenses gives access to the entire project. Also, it is always easier to tag along a running project without having to engage in the fundamental setup," explains CERE Chairman, Erling H. Stenby.

The JIP's are always created with a time horizon of minimum three years, but several of them live much longer. Often the composition of industry partners change over the years as the interest of the companies vary and as some scientific paths show themselves to be more promising than others.

"A company can access and exit a JIP according to the evolvement of its own research strategy. Typically a JIP has an overall generic scope, and the participating companies each define more specific subtasks when they join," Erling H. Stenby notes, adding:

"My experience is that many both industrial and academic partners are attracted by the rather informal atmosphere at CERE. We bring a playful side to energy resources engineering in the sense that we are always open for discussion about new research

programs. Often it is only the challenge that is obvious and we have to develop the ideas for solutions together. This often forms the basis for PhD projects, design of new equipment, or development of new software. We have several examples of that."

The real benefit of these collaborative projects is that all partners wish to find solutions through new scientific insight and by exploring new ideas. We all know that ground breaking research may not lead to the desired answers, but by building long lasting relationships we increase the chance of success and we accumulate knowledge and experience that will guide our further efforts.

The desire to set up projects quickly should never compromise quality, Erling H. Stenby stresses:

"It is extremely important that we can attract talented young scientists for the specific tasks, and that we find the right academic partners for a given project. It is clear that the companies also see the JIPs as a way to recruit new talented coworkers, who are familiar with the most recent developments in their scientific field as well as the applicability to current challenges. Often, the industrial commitment can be combined with public funding, in which case everybody has a valuable leverage of their investment."

**See an overview of the present JIP's and their scope on the following pages.**



### Chemicals for Gas Processing (CHIGP)

Traditionally cubic equations of state have been applied to describe phase equilibria in an oil-gas mixture. Cubic equations of state are relatively simple and hold an outstanding track record within gas-liquid phase equilibria solutions related to oil recovery and other petroleum-related applications. However, current oil recovery and oil transport depends on a range of chemicals needed to facilitate production, i.e. polymers, surface-active substances, emulsion breakers and hydrate inhibitors.

The main purpose of the Chemicals for Gas Processing project (CHIGP) is to develop and maintain a rigorous thermodynamic model, the CPA (Cubic-Plus-Association) equation of state. CPA is a model useful for thermodynamic calculations for mixtures of relevance to the petroleum and chemical industries e.g. mixtures of oil and gas with gas hydrate inhibitors (methanol, glycols) and organic acids.

Such polar and hydrogen bonding compounds are difficult to handle with conventional models and CPA offers a successful alternative and is a good compromise between accuracy and simplicity. The CPA and other tools developed in the project have also proved their worth in other contexts outside the oil industry. Results from CHIGP are disseminated to the participants via CERE's web-site and a special project web-site. The deliverables include software in 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. Moreover, the results are presented in progress meetings held twice per year.

Initiated: 2003.  
Industry partners:  
Current partners are Statoil, GASSCO, BP, Petrobras.  
Coordinator:  
Professor Georgios Kontogeorgis, CERE.

Project web-site: <http://www.chigp.dk>

### Complex Reservoir Simulations (COMPPLEX)

Oil and gas exploration under extreme conditions and the increasing utilization of unconventional resources like oil sand and shale gas have changed the scene for energy resources engineering. Simulations need to address ever more complex phase behaviour. On the positive side, more powerful computers and better algorithms, some of which are developed at CERE by Professor Michael Michelsen's group, have come to the rescue.

COMPPLEX (full title: Compositional Reservoir Simulation Involving Complex Phase Equilibria) is a new JIP dedicated to the field. A top priority will be compositional reservoir simulations that not just calculate average oil properties (so called "black oil simulations") but involve the phase behaviour of the main chemical components of the oil in question. This approach promises far more accurate simulations. Another effort will address the complex phase behaviour seen in carbon dioxide Enhanced Oil Recovery (CO<sub>2</sub> EOR).

Initiated: 2013.  
Industry partners:  
ConocoPhillips, ExxonMobil.  
Coordinator:  
Senior Scientist Wei Yan, CERE.

### Water-based Enhanced Oil Recovery

As the world's oil and gas resources are getting scarcer, novel methods for enhanced oil recovery (EOR) are in high demand. A number of such proposed methods are water-based, and CERE has decided to concentrate efforts that were previously under different labels in this new JIP.

First of all, there is the BioRec program (Biotechnology in Oil Recovery) focussed on both Microbial Enhanced Oil Recovery (MEOR) and enzymatic enhanced oil recovery while also looking into innovative use of biotechnology in relation to prevention of corrosion and gas hydrate formation.

Further, a number of projects runs under the SmartWater program, which investigates flooding techniques with water of different salinity than the reservoir brine. These are water-based EOR techniques and thus included in the new JIP (the geology oriented activities in SmartWater are now a part of the ROCKS project).

The project also contains several elements inherited from the Advanced Oil Recovery Methods (ADORE) project. While officially concluded, the spirit of ADORE, which was to improve understanding of EOR processes, lives on in several current CERE projects.

Initiated: 2013 (built on previous programs BioRec and SmartWater).  
Industry partners:  
Maersk Oil, DONG E&P.  
Coordinator: Associate Professor Alexander Shapiro, CERE.



## Carbon Capture Theme

According to International Energy Agency (IEA) forecasts, global coal consumption will continue at the present level and probably even increase over the next decades. As a means of limiting the contribution of coal to climate change, this has led many countries to take a strong interest in carbon capture and storage (CCS).

Carbon capture is a long standing field of expertise at CERE. We have taken part in a number of European Union research programs – currently we are participating in the OCTAVIUS (Optimization of CO<sub>2</sub> Capture Technology Allowing Verification and Implementation at Utility Scale) project. It is funded under the 7th EU framework program for research (FP7) similar to the newly started INTERACT projects. In INTERACT we are looking at using enzymes to enhance the efficiency of carbon capture solvents. CERE is one of over twenty academic and industrial partners from more than ten countries joined by the common goal of taking CCS closer to industrial application.

CERE has also taken part in the recently concluded European CCS project “iCap”. Here CERE has been active in thermodynamic modeling on two fronts. The first is the idea of utilizing gas hydrates – known to be highly problematic in oil and gas exploration – in carbon capture. The second is the use of complex fluids as de-mixing components.

The following industry partners have participated in collaborative projects in an EU or other context: EON, EDF, EnBW, ESKOM, ENEL, DOOSAN, Gassnova.  
Coordinator:  
Associate Professor Nicolas von Solms, CERE.

## Rock Physics and Rock Mechanics (ROCKS)

Linking rock physics and rock mechanics of sedimentary rocks is a focus area of research in CERE. We cover a wide range of rock types including sandstone, chalk, other carbonate rocks, shale and diatomite. So although we base our research on a solid geological understanding, we see the rocks as representatives of a range of physical properties as porosity, pore size, elasticity and strength.

Rock mechanics addresses the response of a rock in a stress field and quantifies how much elastic deformation in a given stress field is required before pore collapse or failure. The rock is traditionally characterized with respect to mineralogy and petrophysical properties as porosity, pore fluid saturation, and permeability, but we emphasize the role of diagenetic cementation and consequent elasticity.

Rock physics relates elasticity of rocks to their mineralogy, porosity, fluid content and degree of diagenetic cementation. It is traditionally the discipline connecting rock properties with seismics, but in addition to this, we see it as a link between petrophysics and rock mechanics.

The ROCKS project is an extension of NextOil, which is a HPHT (High Pressure, High Temperature) research program in relation to deep oil and gas exploration in the Danish part of the North Sea, where rock physics and rock mechanics play central roles.

Further, the project includes the petrophysical part of the SmartWater program, which investigates advanced water flooding techniques. SmartWater is focussed on two types of sedimentary rocks in the Danish part of the North Sea, chalk and greensand. Samples of both types of rocks are analysed in advanced flooding equipment at CERE.

Initiated: 2013 (built on previous projects NextOil and SmartWater).  
Industry partners:  
DONG E&P and Maersk Oil.  
Coordinator:  
Professor Ida L. Fabricius, CERE.

## Optimizing Oil Production (OPTION)

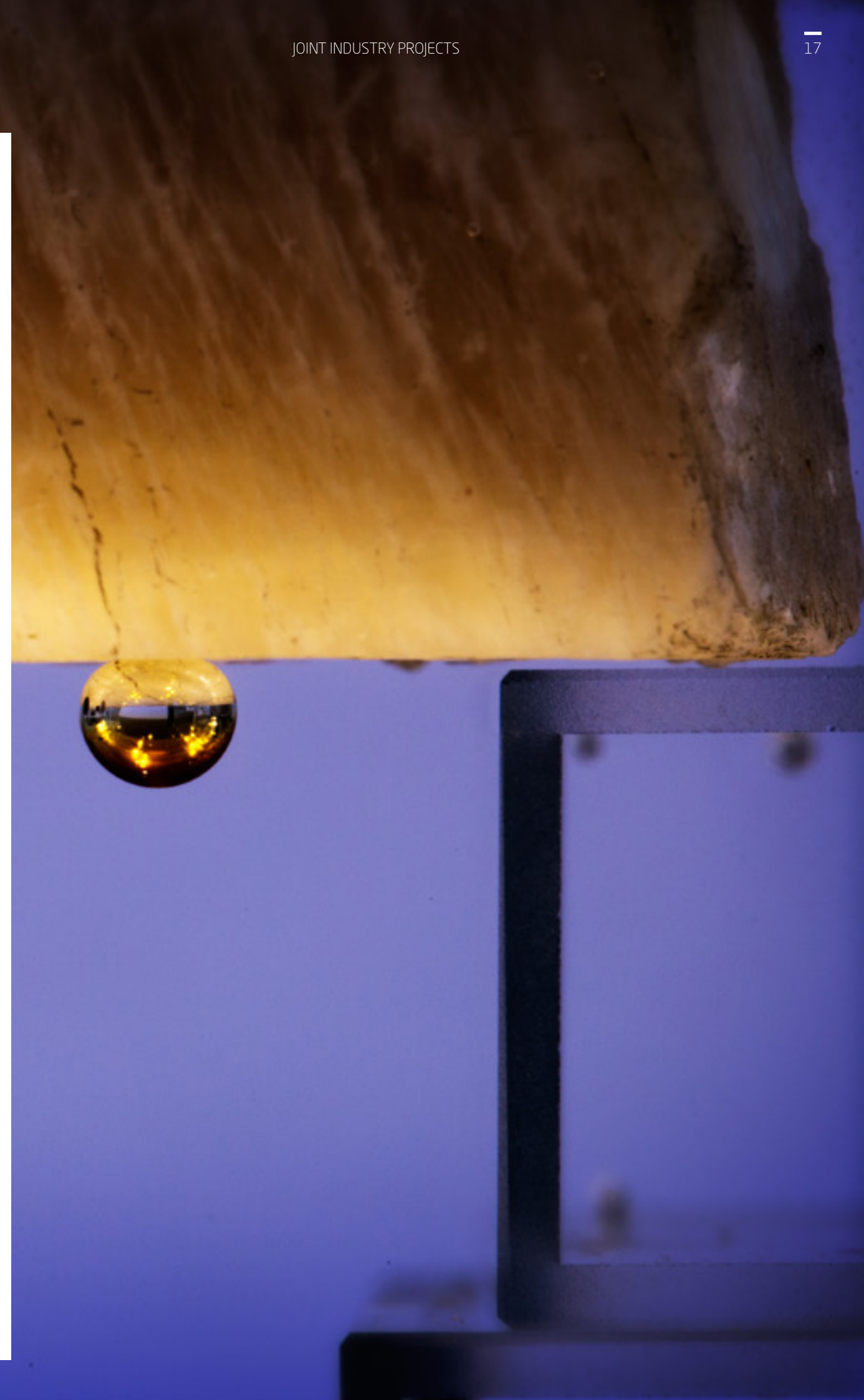
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Various reservoir management regimes have been suggested to maximize oil recovery of a given reservoir. The control input for can be well rates, bottom-hole pressures, valve/choke settings, and others. Typically, the focus is not at maximizing oil production in absolute terms, but rather at maximizing economic gain measured as the value of the oil produced relative to cost of production. In other words the goal is to maximize the net present value of a given oil reservoir over the entire life time of the reservoir.

In the OPTION project such reservoir management regimes are investigated. Further, skills in reservoir modeling, chemical engineering, and computational fluid dynamics (CFD), present at various DTU departments are integrated. Also, quantification of the in-avoidable uncertainties inherent in the found solutions will form a key element in the project.

Initiated: 2013.  
Industry partners:  
Welltec, Lloyd's Register Energy, Senergy.  
Coordinator: Professor Erling H. Stenby, CERE.

Danish National Advanced Technology Foundation press release:  
[http://hoejteknologifonden.dk/nyheder/nyhedsoversigt/investeringer\\_for\\_583\\_mil-lioner\\_kroner\\_starter\\_nye\\_danske\\_teknologieventyr/matematik\\_skal\\_omsaettes\\_til\\_mereolie/](http://hoejteknologifonden.dk/nyheder/nyhedsoversigt/investeringer_for_583_mil-lioner_kroner_starter_nye_danske_teknologieventyr/matematik_skal_omsaettes_til_mereolie/)





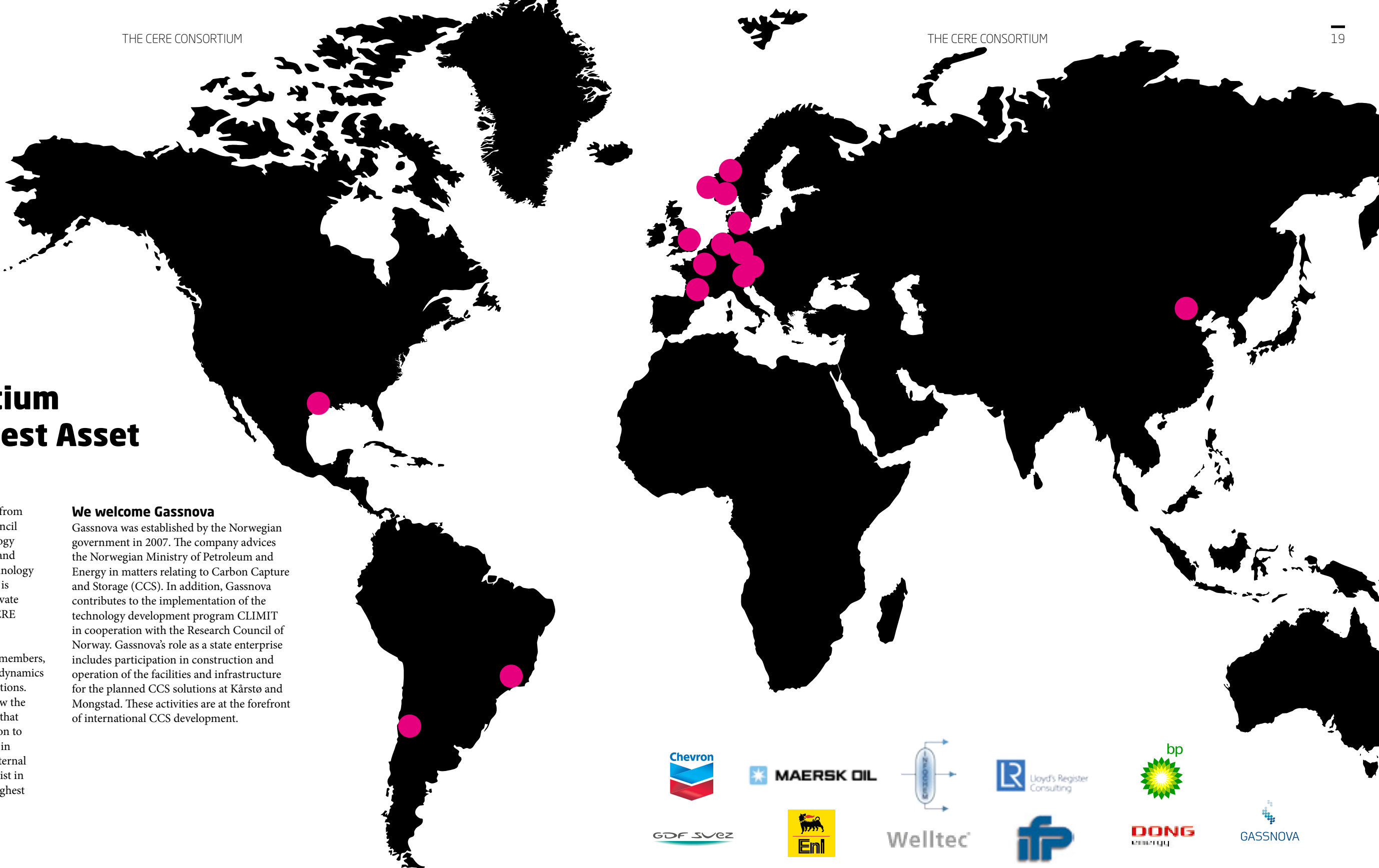
# The Consortium - our Strongest Asset

CERE is supported by public means from several sources, e.g. The Danish Council for Independent Research - Technology and Production Sciences, EU's FP7, and The 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.

Approximately 25-30 companies are members, the exact number changes due to the dynamics of the industry's mergers and acquisitions. The member companies closely follow the activities of the Center. This ensures that CERE activities are relevant in relation to the topical problems and limitations in existing knowledge. This ongoing external control of quality and inspiration assist in maintaining CERE research at the highest international level.

## We welcome Gassnova

Gassnova was established by the Norwegian government in 2007. The company advises the Norwegian Ministry of Petroleum and Energy in matters relating to Carbon Capture and Storage (CCS). In addition, Gassnova contributes to the implementation of the technology development program CLIMIT in cooperation with the Research Council of Norway. Gassnova's role as a state enterprise includes participation in construction and operation of the facilities and infrastructure for the planned CCS solutions at Kårstø and Mongstad. These activities are at the forefront of international CCS development.



# Voices of the CERE Consortium

With 29 industrial Consortium member companies and a high degree of international participation not many other research groups can rival CERE when it comes to industry cooperation.

CERE has always been involved in projects with broad industry applications, often with an international orientation. This is documented by the list of industrial Consortium members. All 29 companies operate on an international scale, and most of them are headquartered outside Denmark.

The relations have evolved over time, and even though CERE has only existed in its present organization for a handful of years, several industry Consortium members have long track records of cooperation.

“We started cooperation at the earlier stages of the IVC-SEP Consortium (the name of the previous organization, which formed the basis for CERE, editors’ remark). I was head of the PVT section of Elf Aquitaine at that time. The agreement was signed in 1981,” recalls Francois Montel, today International Expert at Total which he represents in the Consortium.

“The cooperation is certainly useful for me and my colleagues. It has always been characterized by a good atmosphere and excellent annual meetings,” says Francois Montel.

## Understanding the natural systems

The annual meetings are labelled “Discussion Meetings”. The title underlines that the events are not just about CERE researchers presenting their results to industry. It is a two-way street, meaning that CERE’s management is always looking for input from the Consortium members. Often such input may form the basis for setting up new research projects, sometimes in the form of Joint Industry Projects (JIPs).

“What I like about CERE is that the researchers take time to try to understand the problems of the industry instead of just working on their own projects,” says Dr. Jose Torres of ConocoPhillips.

Originally trained in chemical engineering the present field of Dr. Torres is reservoir simulation. He attended the Discussion Meeting for his first time in 2013:

“I mainly came to learn of new discoveries within classical chemical engineering. In my department we see ourselves as an organization of technology. The ultimate goal is to develop new technology for practical energy engineering. But in order to do that you first need to have a deep understanding of what goes on in the natural systems.”

## A chance to establish a direct relation

Another Discussion Meeting debutant in 2013 was Hussein Alboudwarej of Chevron.

“I find the focus of the event quite wide. Equations of state for aquifers, electrolytes, CPA, PC-SAFT etc. are covered beside the more traditional thermodynamic simulations. Although not directly relevant to my work, it is nice to be introduced to these more advanced models.”

Dr. Alboudwarej was originally trained in chemical engineering and has moved into reservoir simulation during his career at Chevron.

“I have followed the work led by Professors Erling H. Stenby and Michael L. Michelsen from a distance over quite some time. I am glad to have the opportunity to establish a direct relation. Also, I am always interested in obtaining relevant experimental data.”

## Knowing the models - and their limitations

Employed at GDF SUEZ Exploration & Production Germany, Dr. Harm Jan Wubs attended the Discussion Meeting for his third time in 2013:

“I come here to listen. My main interest is what goes on within thermodynamics. Are any new tools available for practical simulations? I am always interested in not only understanding the new tools, but also to learn of their limitations.”

“We do simulations every day, but we should always remember that our results are based not on nature itself, but on models,” Dr. Wubs points out.

“For instance we are often faced with scaling issues. Experiments are done in the lab, and we assume that you can apply the results at much larger scale, but this may not be reality. By attending here I have the chance to learn which fundamental problems are inherent in the various models. This tells me when and where we should be careful.”

## Reflecting developments in industry

Benjamin Sargent of Maersk Oil finds the scientific scope of the Discussion Meeting “quite broad” – which he likes:

“You have topics covered which focus on virtually every part of our business. The thermodynamic section is particularly interesting to us, but I also welcome that CERE has taken up new areas within the geo-disciplines.”

The integration of several disciplines reflects the needs of the industry, Benjamin Sargent feels:

“Our business is very complicated. Reservoirs are becoming harder to find and develop, leading to ever more complex challenges for exploration and production engineers to

solve. And at the same time our products are commodities for which prices fluctuate up and down, leading to changes in the framework conditions for our research and development. All these factors point to a need for integrating several disciplines. At Maersk Oil we already have organized our work within reservoir engineering, geology, and geophysics as one single team.”

## Networking is important

To Dr. Klaus Potsch of Austrian based oil corporation OMV, the 2013 version of CERE’s Discussion Meeting marked a mixture of joy and melancholy:

“I have attended the meeting for many consecutive years, but this was my last event, as I will have retired before next year’s meeting,” he says, summing up his experience with attending over the years:

“I have always had the feeling that I could present problems to the CERE faculty and know that they would actually take time to think about what the solution might be. Networking is obviously a large part of it. I have enjoyed coming here, not just for the science but also on a personal level. I have made many friends over the years.”

## New record in Industry Participation

With 24 companies represented, the 2013 version of CERE’s Discussion Meeting set a new record in industry participation. The annual event is where the center’s industrial Consortium joins CERE researchers to share experiences and exchange ideas.

As always, lengthy sessions during the three-day event were devoted to presentations on the latest developments in thermodynamic modeling and reservoir engineering.

For some years now, academic resources within geology and geophysics have been present in the CERE faculty. Led by Professors Ida Fabricius (geology) and Klaus Mosegaard (geophysics) these two sections contributed strongly to the 2013 event. As a consequence of the broadened scope of CERE, the format was modified, introducing two half-days with parallel sessions rather than keeping the entire agenda in plenum. The parallel sessions were on

Thermodynamics; Enhanced Oil Recovery; Complex Fluid Systems; Geology/Geophysics.

The CERE Discussion Meeting 2013 was held from June 19th – June 21st 2013 at Comwell Borupgaard, Snekkersten. 36 industry participants representing 24 companies and 12 nationalities attended.

Joy and melancholy blended as Dr. Klaus Potsch of OMV attended the Discussion Meeting for the last time in 2013 due to his upcoming retirement.



*“The thermodynamic section is particularly interesting to us, but I also welcome that CERE has taken up new areas within the geo-disciplines.”*

Benjamin Sargent,  
Maersk Oil.



*“What I like about CERE is that the researchers take time to try to understand the problems of the industry.”*

Dr. Jose Torres,  
ConocoPhillips.





# Progress on Dew Points of Natural Gas

Assigned by the European Gas Research Group (GERG), CERE and industry partners have succeeded in combining the thermodynamic model CPA (Cubic-Plus-Association) with standard calculations used in the gas industry.

The water content of natural gas often poses problems during the production, transmission and distribution of the gas. These issues can now be better dealt with through results from a CERE led Joint Industry Project terminated in 2013.

Formally titled “Calculating Dew Points of Natural Gas containing Water and/or selected Production Chemicals” the project is commonly known as GERG, since it was initiated and supported by the European Gas Research Group (GERG). Industry partners were Statoil, GASSCO, Open Grid Europe, DGC, and Snam Rete Gas.

“The water content of natural gas is problematic for several reasons. Small quantities of undesired dissolved water may condense leading to the formation of condensed water, hydrates and/or ice,” explains Professor Georgios Kontogeorgis, CERE, coordinator of the GERG project.

“Such condensed phases may result in corrosion, two-phase flow problems, safety hazards and flow assurance issues, slugging of the flow lines, valves and instrumentation resulting in reduced capacity and shutdowns, and reduction of the oil recovery efficiency because of reduction of the reservoir permeability.”

Accurate thermodynamic models able to calculate the water vapor concentration in equilibrium with hydrate, ice or water in natural gas at pipeline operating conditions (253-323 K and up to 250 bar) are necessary both because experimental data are limited and difficult to obtain, and because the limits of dehydration techniques (usually physical adsorption and condensation) need to be

defined. The latter techniques use chemicals (eg. glycols and alcohols) which also condensate. This adds one more level of modeling challenge.

“The main purpose of the project was to evaluate and compare the performance of the CPA Cubic-Plus-Association equation of state and of the GERG-water calculation method, which is specifically designed to correlate water content and dew points of natural gas,” Georgios Kontogeorgis states.

“The results are directly useable for calculation of dew points of natural gas systems containing water and traces of selected production chemicals.”

Georgios Kontogeorgis,  
Professor, CERE.

“The results are directly useable for calculation of dew points of natural gas systems containing water and traces of selected production chemicals.”

The deliverables include databases of reliable experimental data which will be used to establish and suggest model parameters and modifications, as well as user-friendly software for calculation of dew points and water contents.

Results from the project are disseminated to the participants via CERE's web-site and a special project web-site: <http://gerg.cere.dk>.



# Electron Microscopy to aid Enhanced Oil Recovery

New horizons are opening to the EOR community, as an interdisciplinary project at DTU aims to extend electron microscopy from dry to the complex relevant aqueous samples.

Heterogeneous processes in aqueous environments are of major importance in oil and gas exploration. Besides for the flow of oil and gas in chalk and other types of rock, these processes are relevant for issues like mud filtration around oil wells, precipitation in equipment and others. Moreover, in recent years it has become clear that many of the critical processes need to be looked at on the nanoscale. Therefore Professor Erling H. Stenby, CERE, invited Associate Professor Kristian Mølhave, DTU Nanotech, to engage in a joint effort using Kristian's expertise in imaging at the nanoscale. Obtaining such imaging by electron microscopy is the ambition of the new project called "Nanoscale imaging of aqueous processes of precipitation, dispersion, and imbibition".

For instance, understanding precipitation and imbibition processes involving oil and water in nano- and micrometer sized channels and pores is highly relevant for enhanced oil recovery (EOR). Further, the project will look at nucleation and precipitation processes forming dispersions of particles and slurries

with relevance both for EOR and formation damage.

"We believe to have found a truly new technique for imaging heterogeneous processes in aqueous environments at the nanoscale. We are likely to obtain new fundamental insight once we start imaging these processes in model systems and using relevant samples from industrial collaborators," says Kristian Mølhave.

The project is partly sponsored by the Danish Council for Independent Research - Technology and Production Sciences (FTP).

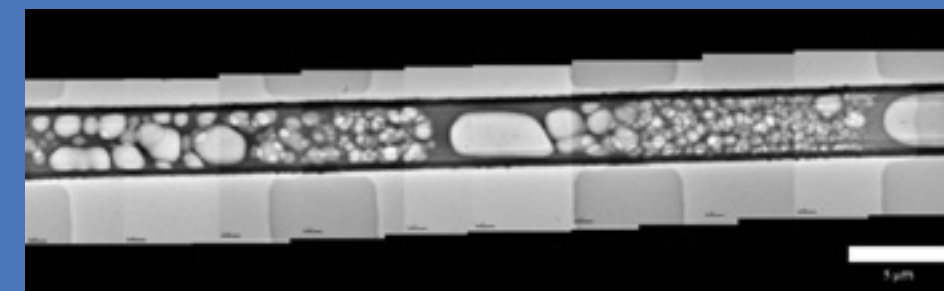
## Frozen membranes on microchips

Involving faculty at DTU Nanotech, CERE, DTU Chemistry, and Center for Electron Nanoscopy (DTU Cen) the project is highly interdisciplinary.

The key point is that as electron microscopes operate under vacuum one cannot just insert an aqueous sample. The trick is either to freeze or to contain the sample somehow, while not disturbing the condition you want to study. In cooperation with DTU Cen Director Andrew Burrows and his group, Kristian Mølhave's group at DTU Nanotech has found a clever approach.

"Just imagine the interest, if we can extend electron microscopy to be generally applicable to aqueous samples and the many complex processes occurring in liquids."

Kristian Mølhave, Associate Professor, DTU Nanotech.



Electron microscopy image showing a micrometer sized channel designed in the project for the study of heterogeneous processes in aqueous environments. Photo: Eric Jensen, DTU Nanotech.

"To study nanoscale processes in water, cryo electron microscopy is typically used to provide the required resolution of a frozen instant in time. Proving images from time series is however a very substantial work," explains Kristian Mølhave.

"In a previous study we have demonstrated that membranes on microchips can be frozen extremely quickly, with freezing rates approaching 1 million Kelvin per second, which is 100 times faster than required to create amorphous ice and hence a well preserved sample with no freezing artifacts. It is highly likely that we can use the techniques for gaining new insight into aqueous processes in aqueous environments."

## New doors for insight

In an ongoing project the group creates suspended microfluidic channels on membranes that promise to be very useful to create frozen samples of for instance shaped Y-channels where two liquids are mixing and to create nanoscale channels. In this way nucleation and imbibition effects in confined regions can be studied. This will open new doors for insight, Kristian Mølhave remarks with enthusiasm:

"Using electron microscopy for imaging of aqueous processes was suggested as early as 1944. But at that time the general state of technology was not up to the task.

The resulting images were not able to compete with ordinary images from optical microscopes. However, some ten years ago the ideas saw a revival."

"Recently there has been almost a revolution in electron microscopy of liquid samples and it will be great to see how that will influence chemistry and other fields. So far, this has been quite limited to dry samples. Just imagine the interest if we can extend electron microscopy to be generally applicable to aqueous samples and the many complex processes occurring in liquids," Kristian Mølhave states.

This is an example of how CERE tries to break new ground as an expansion of its activities.

"We must take risks in order to bring our area of science forward. This project is a totally new direction for us, and I am sure it will have a significant impact if successful" says Erling H. Stenby.



# Optimal Management of Water Flooding



Andrea Capolei, PhD.

Full title: “Non-linear Model Predictive Control for Oil Reservoirs Management.”

Supervisors: John Bagterp Jørgensen, Erling H. Stenby.

Funding: The Danish Council for Independent Research – Technology and Production Sciences.

Water flooding is a standard method for raising oil recovery rates. However, currently water flooding needs to be managed conservatively as a number of uncertainties exist. Thus control regimes that realize a larger proportion of the potential gain promised by water flooding without jeopardizing the stability of the reservoir or the safety of the operation is in high demand. The thesis presents such possible control regimes.

In the primary phase of oil recovery, the reservoir pressure is large enough to make the oil flow to the production wells. In the secondary phase, water must be injected to maintain pressure and move the oil towards the producers. This is known as water flooding.

In the oil industry, closed-loop reservoir management (CLRM) has been suggested to maximize oil recovery of a given reservoir. Typically, the method is not focused at maximizing oil production in absolute terms, but rather at maximizing economic gain

measured as the value of the oil produced relative to cost of production. In other words the goal is to maximize the net present value of a given oil reservoir over the entire life time of the reservoir.

Literature studies show that optimal control strategies may enable higher recovery than conventional water flooding strategies. The control input for CLRM can be well rates, bottom-hole pressures (bhp), valve/choke settings, and others.

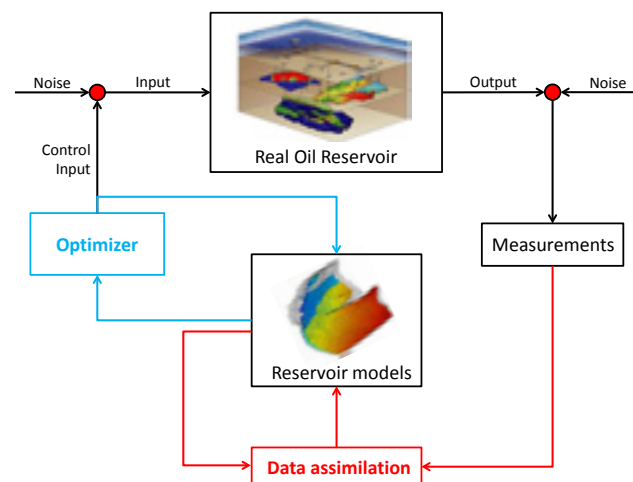
In the project numerical methods for non-linear model predictive control (NMPC) of oil fields was developed. The controller includes a model-based optimizer for maximizing net present value of the reservoir. Further, a parameter and state estimator is included. And finally, use of the moving horizon principle for data assimilation and implementation of the computed control output is implemented.

The controller uses gradient-based optimization and the required gradients are computed by the adjoint method. Use of efficient high order implicit time integration methods for the solution of the forward and the adjoint equations of the dynamical model is proposed. The Ensemble Kalman filter is used for data

assimilation. Further, the use of robust control strategies in both open-loop, i.e. without measurement feedback, and closed-loop, i.e. with feedback, configurations were studied.

The project has three main contributions. Firstly, the computationally expensive gradient computation has been improved by using high-order ESDIRK (Explicit Singly Diagonally Implicit Runge-Kutta) temporal integration methods and continuous adjoints.

Secondly, the Robust Optimization (RO) strategy has been applied in both open-loop and closed-loop configurations. In RO, the water injection and production borehole pressures are computed such that the predicted net present value is maximized. And finally, a mean-variance method for risk mitigation in production optimization of oil reservoirs is presented. Here, a return-risk bi-criterion objective function for the profit-risk tradeoff is introduced. A study focused on open-loop configuration demonstrated that the proposed function is a valuable tool for the profit-risk tradeoff assessment.



Closed loop reservoir management.

# Computer-aided Optimization of Oil Recovery



Katrine Lange, PhD.

Full title: “Inverse Problems in Geosciences: Modeling the Rock Properties of an Oil Reservoir”.

Supervisors: Klaus Mosegaard, Per Christian Hansen, Erling H. Stenby.

Funding: The Danish Council for Independent Research – Technology and Production Sciences.

Currently, Denmark is missing out on approximately 70 % of its North Sea oil, which is trapped in unreachable parts of the reservoirs. Improving the rate of recovery is highly desirable. The thesis focuses on increasing recovery rates of oil reservoirs without costly investments but simply by optimization of the production process. For such optimization two parameters are of high importance. One is the locations and types of the production wells and wells for water or CO<sub>2</sub> injection. The other is the strategy controlling injection and production. Accurate computer models are the foundation for both types of optimization. The thesis focuses on models of spatial parameters describing rock properties of the subsurface using geo-statistical a priori knowledge and available geophysical data.

More specifically, the project proposes a method for efficient and accurate interpolation of rock properties from seismic data. Kriging

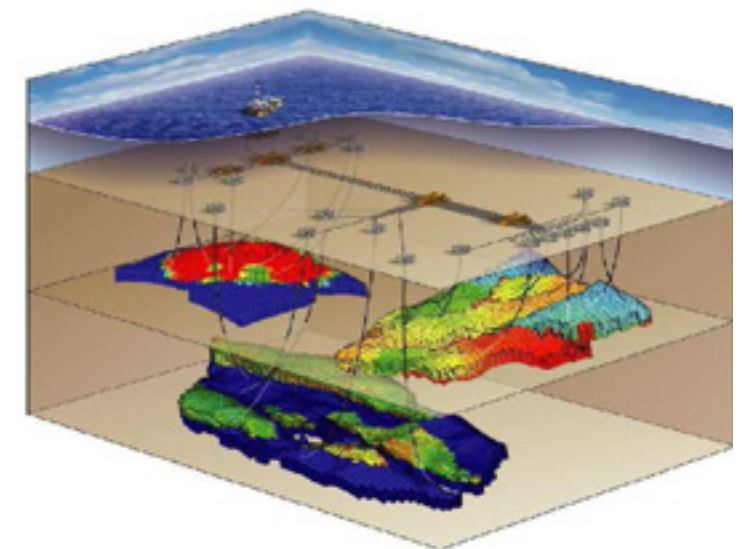
interpolation of a rock property is done in a space spanned by the seismic attributes instead of the traditional approach, which bases the interpolation on spatial coordinates. An orthogonal transformation of the seismic attributes followed by a reduction of dimensions of the interpolation space reduces the computational complexity of the method without significant loss of information.

Further, a closed form expression for an a priori probability density function of a model given multiple-point statistics learned from a training image is formulated. No other existing methods have a closed form expression. Instead they are based on black box routines that can sample the a priori probability density function but not compute relative values of the a priori probability density function between sample models.

Thirdly, the frequency matching method, which enables computing of the maximum a posteriori solution to an inverse problem using multiple-point statistics as prior information, is formulated.

Finally, a general Fortran implementation of the frequency matching method that can be used to solve linear inverse problems, is developed. The implementation is not restricted to a particular application in geosciences, as any training image can be provided and so can the parameters of the linear forward problem.

It should be noted that the objective of the study has been proof of concept rather than solving large-scale, real life problems. Unfortunately, the computational resources of today are not quite adequate for handling the real challenges faced by industry in an ideal fashion. The project is therefore focused on the methods themselves with their potential for future application in mind. However, the study is a first step on the onward journey to incorporate complex geo-statistical prior information to its fullest when solving authentic industry problems.



An offshore oil field. Subsurface reservoirs are connected by wells to units on the seabed again connected to a surface production unit.

# A Probabilistic Approach to Inverse Geo-Problems



Knud Skou Cordua, PhD.

Full title: "Multiple Scenario Generation of Subsurface Models".

Supervisors: Klaus Mosegaard, Ida L. Fabricius.

Funding: DONG E&P.

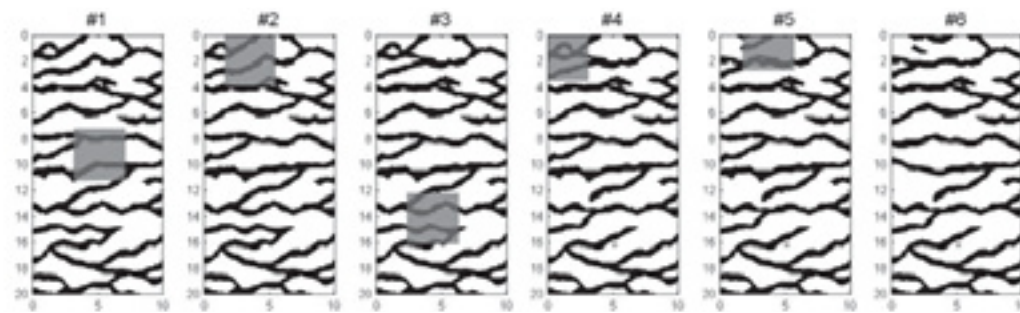
serve the dual purpose of addressing inverse problems while also introducing geological information in a way that enhances the realism of the obtained results.

Traditional solutions to inverse problems are often smooth but without geological realism. The introduction of realistic geological prior information has a regulating effect, allowing reduction of the under-determination in the inverse problem. Moreover, a probabilistic formulation of the inverse problem allows the use of geologically more realistic prior information. Finally, a probabilistic formulation provides a means of analyzing uncertainties and potential multiple-scenario solutions to be used for risk assessments in relation to oil reservoir characterization and forecasting.

Algorithms exist that are able to obtain a sample from the posterior distribution. This is typically necessary in the case of non-linear inverse problems, non-Gaussian prior information, or if the prior information can only be provided through a sampling algorithm. Geo-statistical sampling algorithms based on multiple-point statistics typically use a training image as input and the output is multiple realizations that to some degree honor the multiple-point statistics from the training image.

Oil exploration is one of several disciplines that depend on characterization of the properties and structures of the Earth's subsurface. Much like in astrophysics where we cannot observe the interior of the stars directly, geoscience uses indirect observations in order to obtain information about an unknown system. This leads to inverse problems. The thesis introduces a probabilistic approach that

An example of applying the sequential Gibbs sampler. The dark gray field covers the model parameters that are going to be re-simulated, which is seen by the new structures that occur at this location in the next realization (from Hansen et al., 2012 (paper A2)).



Geo-statistical sampling algorithms that are based on sequential simulation have been investigated. It is found that prior probability distributions that are sampled by such algorithms are not necessarily consistent with training image statistics. However, from Markov random field theory an example of a consistent prior probability distribution is provided. Further, an example of an algorithm that is consistent with the observed statistics from the training image and at the same time takes into account the uncertainty related to the statistics has been proposed.

Common to the methods and strategies presented in this thesis is that they strive for a solution to the inverse problem that is consistent with the available information and to a less degree based on unconscious or subjective choices and implicit assumptions. Future studies related to theoretical developments of these strategies have to be provided. Moreover, applications of these strategies will reveal the practical implications of these consistent formulations. This will in particular be of great importance when it comes to assessments related to cases of high risk such as human health or resources of high economic importance.

# Removal of Impurities from Natural Gas



Negar Sadegh, PhD.

Full title: "Acid Gas Removal from Natural Gas with Alkanolamines: A Modeling and Experimental Study".

Supervisors: Kaj Thomsen, Erling H. Stenby.

Funding: Statoil ASA.

Some 40 % of the world's remaining gas reserves are acidic ("sour"), containing large quantities of CO<sub>2</sub>, and H<sub>2</sub>S and other sulfur compounds. Many large oil and gas fields have more than 10 mole % CO<sub>2</sub> and H<sub>2</sub>S content. As this content is problematic in several ways, various methods for removal of acid gas impurities exist. Most commonly, alkanolamines (simple combinations of alcohol and ammonia) are used as absorption solvents. The thesis focuses on the thermodynamics of such processes, with a special emphasis on the role of pressure, since the absorber pressure is high (around 70 bar), while regenerator pressure is low (1-2 bar).

Different thermodynamic models exist for simulation of acid gas solubility in alkanolamines. However, many of the most used models can give large errors when extrapolated to high pressures, high amine concentrations, mixed solvents, and mixed CO<sub>2</sub> and H<sub>2</sub>O gases. Further, experimental data for high pressures and high amine concentrations are scarce.

The most common alkanolamines for gas treatment are monoethanolamine (MEA), diethanolamine (DEA), methyldiethanolamine (MDEA), and piperazine (PZ). In the modeling part of the project, parameters were determined for a thermodynamic model covering the CO<sub>2</sub>-MDEA-H<sub>2</sub>O, CO<sub>2</sub>-MEA-H<sub>2</sub>O, CO<sub>2</sub>-MDEA-MEA-H<sub>2</sub>O, H<sub>2</sub>S-MDEA-H<sub>2</sub>O, and H<sub>2</sub>S-CH<sub>4</sub>-MDEA-H<sub>2</sub>O systems and the constituent binary subsystems.

The experimental part of the project was carried out at department of Gas Processing and LNG, Research and Development laboratories. A unique set of data for CO<sub>2</sub> solubility in aqueous MDEA at constant total pressure of 110 kPa (1.10 bar), temperatures between 40 to 80 °C and for MDEA concentrations in the range of 10 to 100 mass % were obtained. Density data of MDEA-H<sub>2</sub>O solutions at temperatures between 40 to 80 °C were also acquired.

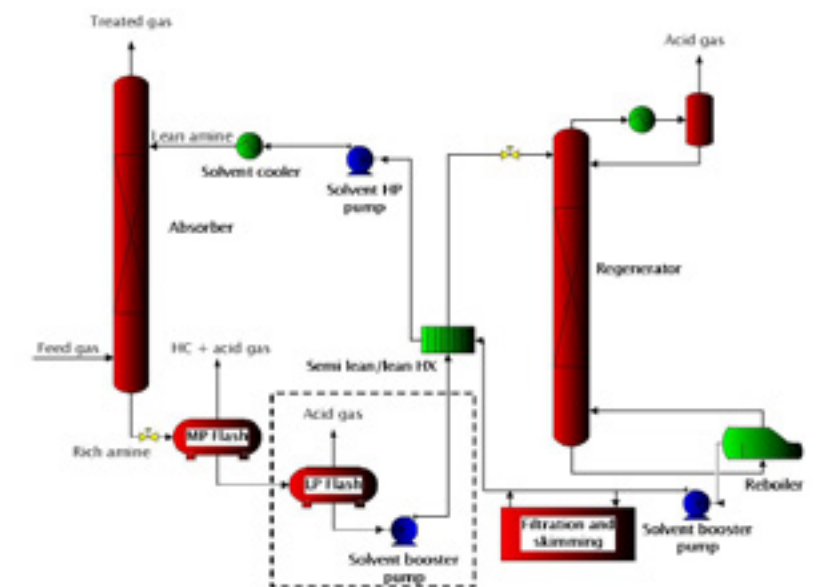
CO<sub>2</sub> solubility was measured in blends of MDEA-PZ at 110 kPa, temperatures between 40 to 70 °C and for MDEA concentrations

ranging from 25 to 75 mass %, while PZ concentration was kept constant at 5 and 10 mass %. The effect of PZ additive was investigated on increasing absorption capacity of aqueous MDEA. Density data of MDEA-PZ-H<sub>2</sub>O solutions at temperatures between 40 and 80 °C were also measured.

Furthermore, the effect of increasing pressure on acid gas solubility was investigated.

Different commercial simulators together with the Extended UNIQUAC model were used to simulate the experimental data points. The effect of total pressure on acid gas solubility was also quantitatively investigated through both experimental and modeling approaches.

Overall, the results show that the thermodynamic model promisingly predict the measured solubility data based on the new model parameters.



The figure shows a typical amine process.



# Modeling of Gas Hydrate based CO<sub>2</sub> Capture



Peter Jørgensen Herslund, PhD.

Full title: "Thermodynamic and Process Modeling of Gas Hydrate Systems in CO<sub>2</sub> Capture Processes."

Supervisors: Nicolas von Solms, Jens Abildskov, Kaj Thomsen.

Funding: The iCAP project (European Union), DTU Chemical and Biochemical Engineering, Otto Mønsted Foundation.

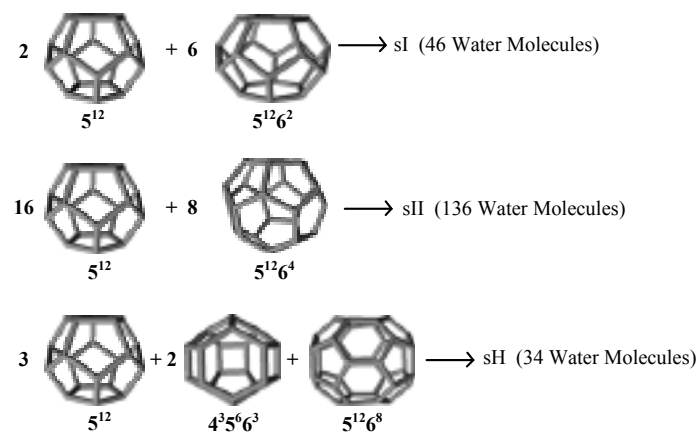
The Copenhagen Agreement founded in 2009 encourages all parties to limit greenhouse gas emission such that the global temperature increase by the year 2100 will be no higher than 2 degrees compared to the pre-industrial level. According to the International Energy Agency (IEA) and other authoritative sources this target can hardly be reached without Carbon Capture and Sequestration (CCS), which is thus an important technological challenge. The thesis focusses on thermodynamic and process modeling of a novel post-combustion technique for carbon capture, namely by gas hydrate formation.

Separation of CO<sub>2</sub> from vapor phases has been done industrially for more than 70 years. A range of methods exist such as physical and chemical absorption, membrane separation and cryogenic separation. However, none of these techniques have yet proven ideal for carbon removal on the very large scale implied by CCS. Especially, the scale of

energy consumption and process equipment investments involved remain too high for broad implementation. Thus, interest in alternative methods remains high. One of these is a gas clathrate hydrate based process, which is the subject of this project.

Gas clathrate hydrates are solid inclusions of sufficiently small molecules physically adsorbed into an ice-like, crystalline lattice of hydrogen bonded water. CO<sub>2</sub> may form gas hydrates with water at a pressure of app. 1.2 MPa and a temperature of 273 K. Separation of CO<sub>2</sub> from flue gases by hydrate formation may be performed at pressures of app. 20 MPa and temperatures below 280 K. As a pressure requirement of this magnitude would make this capture method uncompetitive to existing technologies, thermodynamic promoters are needed. In the project, two well-known thermodynamic promoters, tetrahydrofuran and cyclopentane, were investigated.

A thermodynamic model based on the Cubic-Plus-Association equation of state and the van der Waals-Platteeuw hydrate model is presented. The model enables the performance of a thermodynamic evaluation of gas hydrate forming systems relevant for post-combustion CO<sub>2</sub> capture.



Hydrogen bonded water clusters forming the three most common gas clathrate hydrate structures, sI, sII and sH. Each three-leg intersection point represents an oxygen molecule.

Three to four capture stages are needed in all processes to obtain a product stream richer than 95 mole percent CO<sub>2</sub>. Overall, the modeling results are discouraging, pointing out several drawbacks of using tetrahydrofuran and cyclopentane. Due to their high volatilities they readily transfer to the vapor phases. Furthermore, they lower the process selectivity towards CO<sub>2</sub>, compared to the un-promoted system.

Still, the study produced valuable insight in regards to modeling of gas hydrate based CO<sub>2</sub> capture. It was shown experimentally that the addition of tetrahydrofuran to the ternary system of water-cyclopentane-CO<sub>2</sub> provides an enhanced thermodynamic promotion of the gas hydrate phase. Hydrate equilibrium pressures are reduced by app. 20 percent compared to the cyclopentane system. The mixed promoter system thereby represents a new state-of-the-art within this type of thermodynamic gas hydrate promotion.





# News from CERE

## Advanced Analytical Method based on Radioactive Tracers



Research topics in the SmartWater project, aiming to increase oil and gas recovery rates by use of smart water flooding, has prompted CERE to apply for permission to use advanced analytical methods based on radioactive tracers.

Following the permission for this type of activities, Professor Iver Jakobsen of DTU Chemical Engineering gave a seminar for relevant CERE personnel on the subject “Working with Radioactive Compounds.” The seminar was held September 12, 2013.

## National Research Center for Oil and Gas Research

The challenge of raising recovery rates for oil and gas in the Danish North Sea is now being taken up by a new national research center with its headquarter at DTU.

The new research center will allow Denmark to consolidate its input to improve utilization of the country's oil and gas resources in the North Sea. Today, it is only possible to extract around 28 per cent, on average, of the oil and gas in Danish reservoirs.

The new center is being set up on the basis of an agreement between the Danish government and the Danish Underground Consortium (DUC). DUC partners are

Maersk Oil, Shell, Chevron, and Nordsø-fonden. The DUC partners provide the funding. DTU, Maersk Oil and the other parties in DUC are currently engaged in discussions regarding the establishment process.

The center will not only conduct research, but also provide teaching and training. The overarching goal is to increase the supply of highly qualified people to the Danish oil and gas industry.

The research center will involve researchers from DTU, the University of Copenhagen, Aarhus University, Aalborg University and GEUS. The scientific focus will be on four areas that are crucial to boosting oil and gas recovery in the North Sea: Reservoir modeling, enhanced oil recovery, drilling and production technology, and production facilities and material technology.

It is expected that the center will be officially opened in 2014, and when operating at full capacity it will employ around 100 people.

Source: [www.dtu.dk](http://www.dtu.dk)



## A Korean View on CO<sub>2</sub> Hydrates

The effect of organic matter on the formation kinetics of CO<sub>2</sub> hydrates was the subject of a CERE seminar on May 23, 2013. Associate Professor Woojin Lee of the Korea Advanced Institute of Science and Technology (KAIST) presented results from experiments conducted by his group.



The results indicate that strong binding between soil mineral and organic matter can enhance the hydrate formation kinetics. CO<sub>2</sub> hydrates are highly problematic when they form in production gear during oil and gas production, but they have also been suggested for utilization as a technique for removal of CO<sub>2</sub> from fossil fuel energy production.

## Spotlight on Kinetic Hydrate Inhibition

Peter Englezos, Visiting Professor from University of British Columbia, lectured on “Laboratory evaluation of kinetic hydrate inhibitors” on December 2, 2013. His presentation was both an introduction to major milestones of gas hydrates science and engineering; and also a presentation of recent work at the Department of Chemical and Biochemical Engineering at the University of British Columbia to assess the performance of kinetic hydrate inhibiting molecules.

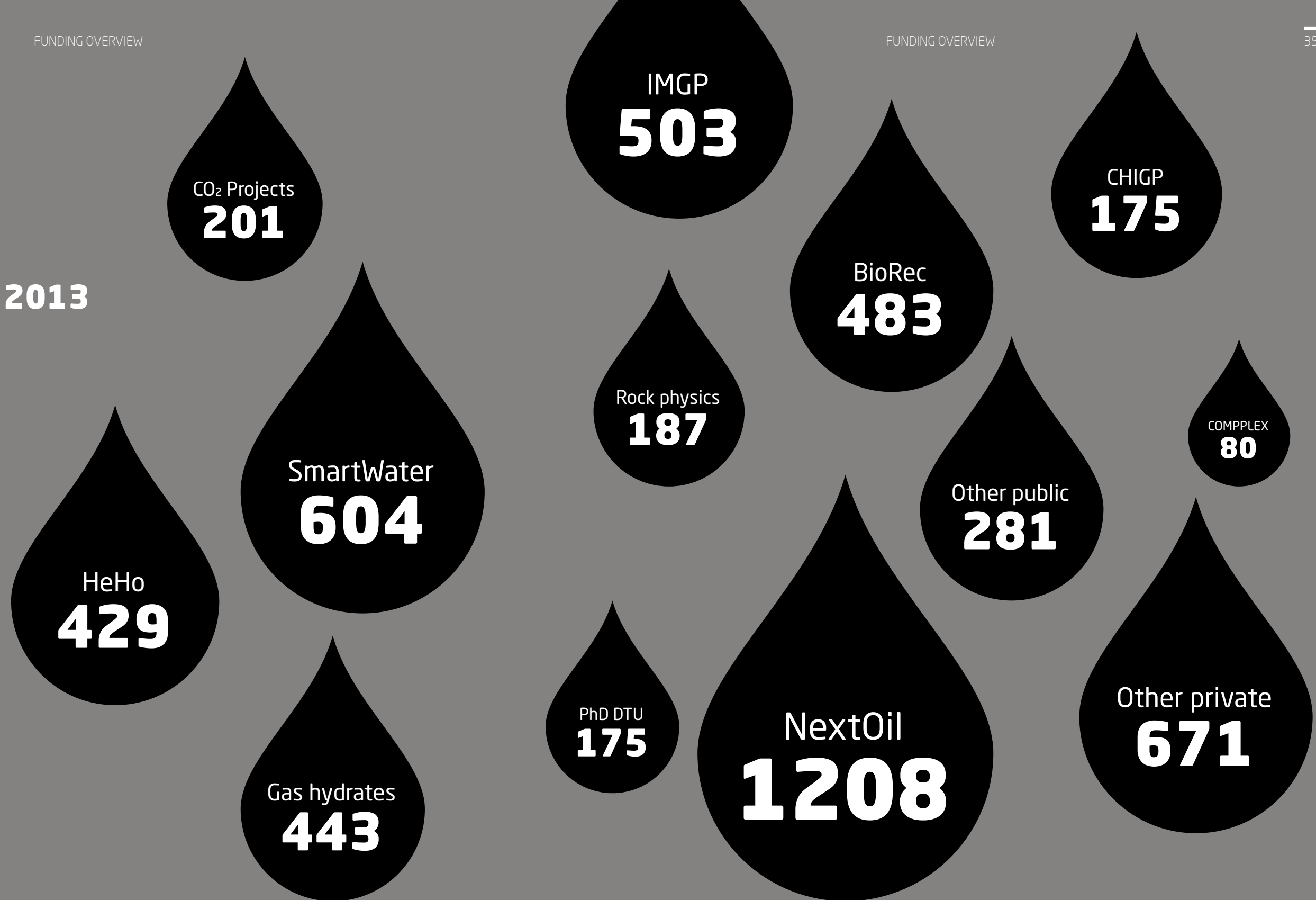


## Research Funding 2013

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 2013 our external funding increased significantly to a total budget of 5.4 million EUR.

The external funding received in 2013 fell under the following projects and categories (all amounts in kEUR):



# Total external funding

# 5440

# Conference Contributions & Invited Speakers

## FEBRUARY

*Thirty-Eighth Workshop on Geothermal Reservoir Engineering, Stanford University, Stanford, California, February 11-13, 2013*

Esther Rosenbrand, Ida Lykke Fabricius, Frans Kets, “Kaolinite mobilisation in sandstone: pore plugging vs suspended particles”, Proceeding of the Thirty-Eighth Workshop on Geothermal Reservoir Engineering, Stanford University, Stanford, California, USA, February 11-13, 2013.12 pages, (oral) <https://pangea.stanford.edu/ERE/pdf/IGAstandard/SGW/2013/Rosenbrand.pdf#>!

*SPE Reservoir Simulation Symposium held in The Woodlands, Texas USA, 18-20 February, 2013*

Abdelkrim Belkadi, Wei Yan, Elsa Moggia, Michael L. Michelsen, Erling H. Stenby, Ivar Aavatsmark, Emanuele Vignati, Alberto Cominelli, "Speeding Up Compositional Reservoir Simulation through an Efficient Implementation of Phase Equilibrium Calculation", SPE Reservoir Simulation Symposium, The Woodlands, Texas USA, 18-20 February 2013 (oral) Paper SPE 163589

## MARCH

*5th International Week Dedicated to Maths 2013, Thessaloniki, Greece, 27-31 March, 2013*

G. M. Kontogeorgis, “Mathematics and Petroleum Engineering”, 5th International Week Dedicated to Maths 2013, Thessaloniki, Greece, 27-31 March, 2013 (Invited Lecture)

*University of Thessaloniki, Greece, 29 March, 2013*

G. M. Kontogeorgis, “Thermodynamics and Energy-related research at DTU Chemical Engineering”, University of Thessaloniki, Greece, 29 March, 2013 (Invited Lecture)

## APRIL

*9th European Federation of Chemical Engineering (EFCE), The Hague, Netherlands, 21-25 April, 2013*

M. Mattei, P. Krogh, B. Depner, G.M. Kontogeorgis, R. Gani, “Design of a Tank Cleaning Blend through a Systematic Emulsified Product Design Methodology”, ECCE 2013, Den Haag, The Netherlands, 21 – 25 April, 2013 (oral)

Nagu Daraboina, Christine Malmos, Nicolas von Solms, “Enhanced Kinetic Inhibition of Natural Gas Hydrate Formation”, 9th European Federation of Chemical Engineering (EFCE), The Hague, Netherlands, April 21-25, 2013 (oral)

## MAY

*Vision Day 2013, DTU Department of Applied Mathematics and Computer Science, 22 May, 2013*

K. Mosegaard, "Imaging and Inversion in Geoscience", Vision Day 2013, DTU Compute, Department of Applied Mathematics and Computer Science, 22 May 2013 (Invited Lecture)

*5th International Conference on Porous Media, PRAGUE, Czech Republic, 22-24 May, 2013*

Esther Rosenbrand, H.D. Holmslykke, M. Olivarius, R. Weibel, M.L. Hjuler, C. Kjøller, Ida L. Fabricius, “The Effect of Kaolinite on the Permeability of the Gassum Sandstone”, 5th International Conference on Porous Media, Prague, Czech Republic, 22-24 May, 2013 (poster)

*Properties and Phase Equilibria for Product and Process Design, Iguazu Falls, Argentina-Brazil, Maj 26-30, 2013*

B. Maribo-Mogensen, G M Kontogeorgis, K Thomsen, "Modeling of Dielectric Properties with an Associating Equation of State",

Properties and Phase Equilibria for Product and Process Design, Iguazu Falls, Argentina-Brazil, Maj 26-30, 2013 (poster)

M. Mattei, G.M. Kontogeorgis, R. Gani, “Development of a Comprehensive Framework for Surfactant Selection and Design for Emulsion Based Chemical Product Design”, PPEPPD 2013, Iguazu Falls, Argentina-Brazil, 26-30 May, 2013 (poster)

Nagu Daraboina, Christine Malmos, Nicolas von Solms, “Experimental Evaluation of the Efficacy of Ice Structuring Proteins as Natural Gas Hydrate Inhibitors”, Properties and Phase Equilibria for Product and Process Design, Iguazu Falls, Argentina-Brazil, May 26-30, 2013 (poster)

*CCS Conference, Antwerp, Belgium, 28-29 May, 2013*

Muhammad Waseem Arshad, Nicolas von Solms, Hallvard Fjøsne Svendsen, Kaj Thomsen, “Thermodynamics of Phase Change Solvents”, CCS Conference, Antwerp, Belgium, 28-29 May, 2013 (oral)

## JUNE

*7th Trondheim CCS Conference (TCCS-7), Trondheim, Norway, 5-6 June, 2013*

Ardi Hartono, Fahad Saleem, Muhammad Waseem Arshad, Hallvard Fjøsne Svendsen, “Binary VLE of DEEA/H<sub>2</sub>O, MAPA/H<sub>2</sub>O and DEEA/MAPA Systems”, 7th Trondheim CCS Conference (TCCS-7), Trondheim, Norway, 4-6 June 2013 (oral)

E. N. Mbia, I.L. Fabricius, F. Frykman, C.M. Nielsen, C. Bernstone, G. Pickup, “Caprock Compressibility and the Consequences for Pressure Development in CO<sub>2</sub> Storage Sites, 7th Trondheim CCS Conference (TCCS-7), 4-6 of June 2013 in Trondheim, Norway (oral)

Jozsef Gaspar, Kaj Thomsen, Nicolas von Solms, Philip Loldrup Fosbøl, “Interfacing Absorber and Desorber Columns for CO<sub>2</sub>

Post-combustion Modelling”, TCCS-7, Trondheim, Norway, June 4-6, 2013 (poster)

Muhammad Waseem Arshad, Philip Loldrup Fosbøl, Nicolas von Solms, Hallvard Fjøsne Svendsen, Kaj Thomsen, “Equilibrium Solubility of CO<sub>2</sub> in Alkanolamines”, 7th Trondheim CCS Conference (TCCS-7), Trondheim, Norway, 5-6 June, 2013 (poster) (To be published in Energy Procedia)

*ESCAPE 2013, Laapenranta, Finland, 9-12 June, 2013*

M. Mattei, M. Hill, G.M. Kontogeorgis, R. Gani, “Design of an Emulsion Based Personal Detergent through a Model Based Chemical Product Design Methodology”, ESCAPE 2013, Laapenranta, Finland, 9-12 June, 2013, published (CACE 32, 2013) (poster)

*75th EAGE Conference & Exhibition incorporation SPE EUROPEC 2013, London, United Kingdom, 10-13 June, 2013*

Alsu Khusainova, Alexander Shapiro, Erling Stenby and John Woodley, “Potential of Enzymes as Enhanced Oil Recovery Agents”, 75th EAGE Conference & Exhibition incorporating SPE EUROPEC 2013, London, United Kingdom, 10-13 June, 2013 (oral) Amalia Halim, Alexander Shapiro, Sidsel Marie Nielsen and Anna Eliasson Lantz, “The Effect of Bacteria Penetration on Chalk Permeability”, 75th EAGE Conference & Exhibition incorporation SPE EUROPEC 2013, London, United Kingdom, 10-13 June, 2013 (oral)

A. Awadalkarim, I. L. Fabricius, “Petrophysical Analysis of Siliceous Ooze Sediments, Møre Basin, Norwegian Sea” In: Proceedings of the 75th EAGE Conference & Exhibition incorporating SPE EUROPE 2013, London, United Kingdom, 10–13 June 2013. Expanded abstract We 09 07, 4 pages (oral) I. L. Fabricius, “Calculating Vertical Stress in Chalk” In: Proceedings of the 75th EAGE Conference & Exhibition incorporating SPE

EUROPE 2013, London, United Kingdom, 10–13 June 2013. Expanded abstract H06, 2 pages (oral)

K. Katika, M. M. Alam, I. L. Fabricius, ”Nuclear Magnetic Resonance and Elastic Wave Velocity of Chalk Saturated with Brines Containing Divalent Ions. Paper presented at 75th EAGE Conference & Exhibition incorporating SPE EUROPEC 2013, London, United Kingdom. Expanded abstract We 09 03, 4 pages (oral)

M. M. Alam, K. Katika, I.L. Fabricius, “Wettability of Quartz Surface as Observed by NMR Transverse Relaxation Time (T<sub>2</sub>)”, 75th EAGE Conference & Exhibition incorporating SPE EUROPEC 2013, London, United Kingdom, 10-13 June, 2013, Expanded abstract, We 09 01. 4 pages (oral)

*SIAM Conference on Mathematical & Computational Issues in the Geosciences, Padua, Italy, 17-20 June, 2013*

Michael L. Michelsen, “Calculation of Phase Equilibrium: Status and Perspectives”, SIAM Conference on Mathematical & Computational Issues in the Geosciences, Padua, Italy, 17-20 June, 2013 (oral)

*VIII Hotine Marussi Symposium, Rome, June 17-21, 2013*

K. Mosegaard "Inverse Modeling - With a commemoration of Albert Tarantola", VIII Hotine Marussi Symposium, Rome, 17-21 June, 2013 (Invited Lecture)

*1st International UAM-ECUA Conference and Exhibition on Underwater Acoustics, Corfu, Greece, 23-28 June 2013*

A. Xenaki, P. Gerstoft, K. Mosegaard, "Inversion assuming weak scattering", In proceedings: Proceedings of the 1st International UAM-ECUA Conference and Exhibition on Underwater Acoustics, Corfu, Greece, 23-28 June, 2013 (oral)

## JULY

*5th BIOT Conference on Poromechanics, Vienna, Austria, 10-12, July, 2013*

M. M. Alam, I. L. Fabricius, “Change in Biot’s Effective Stress Coefficient of Chalk during Pore Collapse”, 5th BIOT Conference on Poromechanics, Vienna, Austria, 10-12 July, 2013, ASCE Library Poromechanics V: 2395-2403 (oral)

K. A. Andreassen, I. L. Fabricius, “Poroelasticity of High Porosity Chalk under Depletion”, 5th Biot Conference on Poromechanics, Vienna, Austria, 10-12 July, 2013, ASCE Library, Poromechanics V: 2423-2430 (oral) I. L. Fabricius, M. M. Alam, “Burial Diagenesis of Deep Sea Chalk as Reflected in Biot's Coefficient”, 5.th Biot Conference on Poromechanics, Vienna, Austria, 10-12 July, 2013, ASCE Library, Poromechanics V: 2414-2422 (oral)

K. Katika, M. M. Alam, I. L. Fabricius, ”Nuclear Magnetic Resonance and Sound Velocity Measurements of Chalk Saturated with Magnesium Rich Brine”, 5.th Biot Conference on Poromechanics, Vienna, Austria, 10-12 July, 2013, ASCE Library, Poromechanics V: 678-684 (oral)

M. K. Sørensen, I. L. Fabricius, “Quantifying the Effect of Squirt Flow Dispersion from Compliant Clay Porosity in Clay Bearing Sandstones”, 5.th Biot Conference on Poromechanics, Vienna, Austria, 10-12 July, 2013, ASCE Library, Poromechanics V: 249-258. (oral)

## AUGUST

*2nd international Workshop on Rock Physics, Southampton, United Kingdom, 4-9 August, 2013*

I. L Fabricius, “Burial Stress on Carbonate Rocks”, 2nd international workshop on Rock Physics, Southampton, United Kingdom, 4-9

August, 2013, Book of abstracts 77-80 (oral)  
J. Regel, J. K. A. Andreassen, I. L. Fabricius, “Example of Effect on Calculated Biot’s Coefficient under HTHP Conditions”, 2nd international workshop on Rock Physics, Southampton, United Kingdom, 4-9 August, 2013, Book of abstracts 81-84. (oral)

M. K. Sørensen, I. L. Fabricius, “Modulus Changes Caused by Pore-fillings Clays in Partially Saturated Sandstones”, 2nd International Workshop on Rock Physics, Southampton, United Kingdom, 4-9 August, 2013, Book of abstracts 140-143. (oral)

*4th International Symposium on Applied Microbiology and Molecular Biology (ISMOS-4), Rio de Janeiro, Brazil, 24-28 August 2013*

Amalia Halim, Dorthe Skou Pedersen, Anna Eliasson Lantz, Sidsel Marie Nielsen and Alexander Shapiro, “Molasses injection as a MEOR strategy: Enrichment incubations of brine/oil from North Sea Oil Field”, 4th International Symposium on Applied Microbiology and Molecular Biology (ISMOS-4), Rio de Janeiro, Brazil, 24-28 August 2013 (poster)

SEPTEMBER

*15th Annual Conference of the International Association for Mathematical Geosciences (IAMG 2013), Madrid, Spain, 2-6 September, 2013*

Y. Melnikova, K. Lange, A. Zunino, K. S. Cordua, K. Mosegaard, "History Matching with Geostatistical Prior: a Smooth Formulation", In: Mathematics of Planet Earth, Lecture Notes in Earth System Science 2013, pp 703-707, Proc. of the 15th Annual Conference of the International Association for Mathematical Geosciences (IAMG 2013), Madrid, Spain, 2-6 September, 2013 (oral)

A. Zunino, K. Lange, Y. Melnikova, T. M. Hansen, K. Mosegaard, "Reservoir modeling

combining geostatistics with Markov chain Monte Carlo inversion". In: Mathematics of Planet Earth, Lecture Notes in Earth System Sciences, pp 683-687. Proc. of the 15th Annual Conference of the International Association for Mathematical Geosciences (IAMG 2013), Madrid, Spain, 2-6 September, 2013 (oral)

*Thermodynamics 2013, Manchester, United Kingdom, 3-6 September 2013*

B. Maribo-Mogensen, G M Kontogeorgis, K Thomsen, "The Electrolyte CPA Equation of State", Thermodynamics 2013, Manchester, United Kingdom, 3-6 September 2013 (oral)

B. Maribo-Mogensen, G M Kontogeorgis, K Thomsen, "Modeling of Dielectric Properties with an Associating Equation of State", Thermodynamics 2013, Manchester, United Kingdom, 3-6 September 2013 (poster)

Kontogeorgis, G.M., “Thirty Years with Association Models – what have we learnt?”, Thermodynamics 2013, Manchester, United Kingdom, 3-6 September 2013 (oral)

Martin G. Bjørner and Georgios M. Kontogeorgis, “An Engineering Equation of State Contribution for Quadrupolar Fluids”, Thermodynamics 2013, Manchester, United Kingdom, 3-6 September, 2013 (5 min presentation)

Martin G. Bjørner and Georgios M. Kontogeorgis, “An Engineering Equation of State Contribution for Quadrupolar Fluids”, Thermodynamics 2013, Manchester, United Kingdom, 3-6 September, 2013 (poster)

M. Frost, G M Kontogeorgis, N. von Solms, "Measurement and Modeling of Phase Equilibrium of systems containing Polar Chemicals", Thermodynamics 2013, Manchester, United Kingdom, 3-6 September 2013 (15min oral)

Xiaodong Liang, and Georgios Kontogeorgis, “Comparison of the Pure Component

Parameters of Water with the Simplified PC-SAFT EOS”, Thermodynamics 2013, Manchester, United Kingdom, 3-6 September, 2013 (poster)

*IEA EOR 34th Annual Symposium, Stavanger, Norway, 8-12 September, 2013*

Sidsel Marie Nielsen, Amalia Halim, Igor Nesterov, Anna Eliasson Lantz, Alexander Shapiro, Erling Stenby, "Microbial Enhanced Oil Recovery: The Potential of Spore-forming Bacteria", IEA EOR 34th Annual Symposium, Stavanger, Norway, 8-12 September, 2013 (oral)

Wei Yan, Michael L. Michelsen, Erling H. Stenby, "Negative Flash for Calculating the Intersecting Key Tie-lines in the MOC Solution of Gas Injection" IEA EOR 34th Annual Symposium, Stavanger, Norway, 8-12 September 2013 (oral)

*2nd Post Combustion Capture Conference (PCCC2), Bergen, Norway, 17-20 September, 2013*

Muhammad Waseem Arshad, Philip Loldrup Fosbøl, Nicolas von Solms, Hallvard Fjøsne Svendsen, Kaj Thomsen, “Vapor-Liquid Equilibrium of CO2 with Aqueous Solutions of DEEA, MAPA and Their Mixture”, 2nd Post Combustion Capture Conference (PCCC2), Bergen, Norway, 17-20 September (oral)

Hanne M. Kvamsdala, Sören Ehlers, Purvil Khakharia, Philip Loldrup Fosbøl, Ulrich Liebenthal, Cristina Sanchez Sanchez, Geir Haugen, Actor Chikukwa, Laurence Robinson, Nick Booth, Adrien Gomez, Fabrice Chopin, “A New Reference Case for Benchmarking in the OCTAVIUS project”, 2nd Post Combustion Capture Conference (PCCC2), Bergen, Norway, 17-20 September (oral)

*CAPE-OPEN Annual Meeting, Lyon, France 18-19 September, 2013*

B. Maribo-Mogensen, G. M. Kontogeorgis, "Dissemination of University Research Through CAPE-OPEN", CAPE-OPEN Annual Meeting, Lyon, France, 18-19 September (oral)

*83th Annual Meeting of the Society of Exploration Geophysicists, Houston, USA, 22-27 September, 2013*

M. M. Alam, K. Katika, I. L. Fabricius, “Effect of Dissolved Ions on Bound Water on Water Wet Mineral Surfaces as indicated by NMR Transverse Relaxation Time (T2)”, 83th Annual Meeting of the Society of Exploration Geophysicists, Houston, USA, 22-27 September, 2013, SEG Technical Program Expanded Abstracts 2013: 2732-2736 (oral)

A. S. Johansen, T. M. Hansen, I. L. Fabricius, “Rock Physics Based Non-linear AVO Waveform Inversion of North Sea Greensand”, 83th Annual Meeting of the Society of Exploration Geophysicists, Houston, USA, 22-27 September, 2013, SEG Technical Program Expanded Abstracts 2013: 3139-3143 (oral)

*Oceans 2013 IEEE, San Diego, USA, 23-26 September, 2013*

A. Xenaki, P. Gerstoft, O. Carriere, K. Mosegaard, "Statistical Characterization of Weak Scattering Fields with Inverse Methods": In proceedings: Oceans 2013 IEEE, San Diego, USA, 23-26 September, 2013 (oral)

OCTOBER

*Workshop Mathematiques pour La Planete Terre, Université de Lorraine, Fédération Charles Hermite, Nancy, France, 9-10 October, 2013*

K. Mosegaard, "The Complex Earth", Workshop Mathematiques pour La Planete Terre, Université de Lorraine, Fédération Charles Hermite, Nancy, France, 9-10 October, 2013 (Invited Lecture)

*Aalto University, Aalto, Finland, 11 October, 2013*

Kontogeorgis, G.M., “Modeling of complex phase behavior with the CPA Equation of State”, Aalto University, Aalto, Finland, 11 October, 2013 (Invited Lecture)

NOVEMBER

*AICHE Annual Meeting, San Francisco, USA, 3-8 November, 2013*

B. Maribo-Mogensen, G. M. Kontogeorgis, "Dissemination of University Research Through CAPE-OPEN", AIChE Annual Meeting, San Francisco, USA, 3-8 November, 2013 (oral)

B. Maribo-Mogensen, G. M. Kontogeorgis, K. Thomsen, "Modeling of Thermodynamic, Volumetric, and Electrical Properties with the Electrolyte CPA Equation of State", AIChE Annual Meeting, San Francisco, USA, 3-8 November, 2013 (poster)

B. Maribo-Mogensen, G. M. Kontogeorgis, K. Thomsen, "Modeling of Dielectric Properties of Complex Fluids With the Electrolyte CPA Equation of State", AIChE Annual Meeting, San Francisco, USA, 3-8 November, 2013 (poster)

Christine Malmos, Pei Cheng Chua, Nagu Daraboina, Dennis Friis, Erlend Kristiansen, Hans Ramløv, John M. Woodley, Malcolm Kelland, Nicolas von Solms, “Inhibition of Gas Hydrate Formation With a Hyperactive Insect Antifreeze Protein”, AIChE Annual Meeting, San Francisco, USA November 3-8, 2013 (oral)

G. M. Kontogeorgis, “Thirty Years With Association Models – What Have We Learnt?”, AIChE Annual Meeting, San Francisco, USA, 3-8 November, 2013 (oral)

Nagu Daraboina, Nicolas von Solms, “CO<sub>2</sub> Capture by Gas Hydrate Formation:

Combined Effect of Thermodynamic and Kinetic Promoters”, AIChE Annual Meeting, San Francisco, USA 3-8 November, 2013 (oral)

M. Mattei, G. M. Kontogeorgis, R. Gani, “Predicting Surfactant Related Properties for Chemical Based Product Design”, AIChE Annual Meeting 2013, San Francisco, USA, 3-8 November, 2013 (oral)

M. Mattei, G. M. Kontogeorgis, R. Gani, “Use of Water-Oil-Surfactant System Phase Behavior Data/Models for Emulsion Based Chemical Product Design”, AIChE Annual Meeting 2013, San Francisco, USA, 3-8 November, 2013 (oral)

*EAGE/SPE Joint Workshop 2013 "Beyond Closed Loop Integrated Monitoring", Lisbon, Portugal, 17-20 November, 2013*

Y. Melnikova, A. Zunino, K. Lange, K. S. Cordua, K. Mosegaard, “History Matching Problem with Geostatistical Priors in a Smooth Formulation”, EAGE/SPE Joint Workshop 2013 "Beyond Closed Loop Integrated Monitoring", Lisbon, Portugal, 17-20 November, 2013 (oral)



# Master Theses 2013

**Jordi Brull Costa**  
“Polymers as barrier membranes in pipelines for supercritical CO<sub>2</sub> in offshore applications”

**Tobias Gram**  
“Analysis of elasticity and compaction data for North Sea chalk”

**Casper Eastgate**  
“Viscosity Modeling of Asymmetric Mixtures in Oil and Gas Production”

**Anette Lunde**  
“Application of enzymes for enhanced oil production”

**Jeppe Bendix Regel**  
“Rock physical interpretation of logs from Hejre field”

**Nathaniel Denis John Simpson**  
“Fracture growth in anisotropic rock”

**Chaudhary Bilal Shaukat**  
“Effect of salinity on waterflooding of petroleum reservoirs”

**Lykourgos Sigalas**  
“Effect of salinity on waterflooding of petroleum reservoirs”

**Søren Dejgaard Schmidt**  
“Modeling of mineral scale deposition in oil production”

**Phillip Mutebi Wolf**  
“Experimental determination of solid formation from CO<sub>2</sub> capture solvents”



# Publications 2013

## Previously submitted manuscripts

<b>CERE 1030</b>	<i>“Composition of In Situ Burn Residue as a Function of Weathering Conditions”</i>  J. Fritt-Rasmussen, B.E. Ascanius, P.J. Brandvik, A. Villumsen, and E.H. Stenby, (Marine Pollution Bulletin, 67 (2013) 75-81)
<b>CERE 1208</b>	<i>“Evaluation of the PC-SAFT, SAFT and CPA equations of state in predicting derivative properties of selected non-polar and hydrogen-bonding compounds”</i>  A.J. de Villiers, C.E. Schwarz, A.J. Burger, and G.M. Kontogeorgis (Fluid Phase Equilibria, 338 (2013) 1-15)
<b>CERE 1213</b>	<i>“A New Pilot Absorber for CO2 Capture from Flue Gases: Measuring and Modelling Capture with MEA Solution”</i>  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)
<b>CERE 1224</b>	<i>“Distribution of MEG and Methanol in Well-defined Hydrocarbon and Water Systems: Experimental Measurement and Modeling using the CPA EoS”</i>  Muhammad Riaz, Mustafe A. Yussuf, Georgios M. Kontogeorgis, Erling H. Stenby, Wei Yan, and Even Solbraa (Fluid Phase Equilibria, 337 (2013) 298-310)
<b>CERE 1230</b>	<i>“Potential Theory of Adsorption for Associating Mixtures: Possibilities and Limitations”</i>  Martin G. Bjørner, Alexander A. Shapiro, and Georgios M. Kontogeorgis (Industrial & Engineering Chemistry Research, 52(7) (2013) 2672-2684)

<b>CERE 1233</b>	<i>“Thermodynamic Modelling of Natural Gas Systems Containing Water”</i>  Eirini K. Karakatsani, and Georgios M. Kontogeorgis (Industrial & Engineering Chemistry Research, 52 (2013) 3499-3513)
<b>CERE 1234</b>	<i>“Modeling of Dielectric Properties of Complex Fluids with an Equation of State”</i>  Bjørn Maribo-Mogensen, Georgios M. Kontogeorgis, and Kaj Thomsen (J. Chem. Phys. B, 117(12) (2013) 3389-3397)
<b>CERE 1235</b>	<i>“GC-PPC-SAFT Equation of State for VLE and LLE of Hydrocarbons and Oxygenated Compounds. Sensitivity Analysis.”</i>  Thanh-Binh Nguyen, Jean-Charles de Hemptinne, Benoit Creton, and Georgios M. Kontogeorgis (I&EC Research, 52 (2013) 7014-7029)

## New manuscripts

<b>CERE 1301</b>	<i>“Solids Modelling and Capture Simulation of Piperazine in Potassium Solvents”</i>  Philip Loldrup Fosbøl, Bjørn Maribo-Mogensen, and Kaj Thomsen (Presented at the International Conference on Greenhouse Gas Technologies (GHGT), Kyoto, Japan, 18-22 November 2012) (Submitted for publication)
<b>CERE 1302</b>	<i>“Alternative Layouts for the Carbon Capture with the Chilled Ammonia Process”</i>  Gianluca Valenti, Davide Bonalumi, Philip Fosbøl, Ennio Macchi, Kaj Thomsen, and Domenico Gatti (Presented at the International Conference on Greenhouse Gas Technologies (GHGT), Kyoto, Japan, 18-22 November 2012) (Submitted for publication)

<b>CERE 1303</b>	<i>“Improved Population Balance Model for Straining-dominant Deep Bed Filtration using Network Calculations”,</i> Hao Yuan, Zhenjiang You, Alexander Shapiro, and Pavel Bedrikovetsky (Chemical Engineering Journal, 226 (2013) 227-237)
<b>CERE 1304</b>	<i>“Association Models for Petroleum Applications”</i>  G.M. Kontogeorgis (Vestnik (Herald) of St. Petersburg State University, Ser. 4 (Physics, Chemistry), Issue 1, March 2013, pp. 63-79)
<b>CERE 1305</b>	<i>“Liquid-Liquid Equilibria for Reservoir Fluids + Monoethylene Glycol and Reservoir Fluids + Monoethylene Glycol + Water: Experimental Measurements and Modeling using the CPA EoS”</i>  Michael Frost, Georgios M. Kontogeorgis, Erling H. Stenby, Mustafe A. Yussuf, Toril Haugum, Kjersti O. Christensen, Even Solbraa, and Torbjørn V. Løkken (Fluid Phase Equilibria, 340 (2013) 1-6)
<b>CERE 1306</b>	<i>“Capabilities and Limitations of Predictive Engineering Theories for Multicomponent Adsorption”</i>  Sofie Bartholdy, Martin G. Bjørner, Even Solbraa, Alexander Shapiro, and Georgios M. Kontogeorgis (Industrial and Engineering Chemistry Research, 52 (33) (2013) 11552-11563)
<b>CERE 1307</b>	<i>“Vapor-Liquid-Liquid Equilibrium Measurements and Modeling of Ethanethiol plus Methane plus Water, and 1-butanethiol plus Methane plus Water Ternary Systems at 303, 335 and 365 K and Pressure up to 9 MPa”</i>  Javeed Awan, Georgios M. Kontogeorgis, Ioannis Tsivintzelis, and Christophe Coquelet (Ind. Eng. Chem. Res., 52(41) (2013) 14698-14705)

<b>CERE 1308</b>	<i>“Ionic Networks Derived from the Protonation of Dendritic Amines with Carboxylic Acid End-Functionalized PEGs”</i>  Lidia González, Anne Ladegaard Skov, and Søren Hvilsted (Journal of Polymer Science, Part A: Polymer Chemistry, 51 (2013) 1359-1371)
<b>CERE 1309</b>	<i>“A Theoretical Analysis of Colloid Attachment and Straining in Chemically Heterogeneous Porous Media”</i>  Scott A. Bradford, Saeed Torkzaban, and Alexander Shapiro (Langmuir, 29 (2013) 6944-6952)
<b>CERE 1310</b>	<i>“Modeling of Dielectric Properties of Aqueous Salt Solutions with an Equation of State”</i>  Bjørn Maribo-Mogensen, Georgios M. Kontogeorgis, and Kaj Thomsen (The Journal of Physical Chemistry, 117 (2013) 10523-10533)
<b>CERE 1311</b>	<i>“Experimental Study of Bacterial Penetration into Chalk Rock: Mechanisms and Effect on Permeability”</i>  Amalia Halim, Alexander Shapiro, Anna Eliasson Lantz, and Sidsel Marie Nielsen (Accepted for publication in Transport in Porous Media Journal)
<b>CERE 1312</b>	<i>“Modeling of the Critical Micelle Concentration (CMC) of Nonionic Surfactants with an Extended Group-Contribution Method”</i>  Michele Mattei, Georgios M. Kontogeorgis, and Rafiqul Gani (Industrial & Engineering Chemistry Research, 52 (2013) 12236-12246))



# Publications 2013

## New manuscripts

<b>CERE 1313</b>	<i>“Synergistic Inhibition of Natural Gas Hydrate Formation”</i>  Nagu Daraboina, Christine Malmos, and Nicolas von Solms (Fuel, 108 (2013) 749-757)
<b>CERE 1314</b>	<i>“SIPPI: A Matlab Toolbox for Sampling the Solution to Inverse Problems with Complex Prior Information – Part I”</i>  Thomas Mejer Hansen, Knud Skou Cordua, Majken Caroline Looms, and Klaus Mosegaard (Computers & Geosciences, 52 (2013) 470-480)
<b>CERE 1315</b>	<i>“SIPPI: A Matlab Toolbox for Sampling the Solution to Inverse Problems with Complex Prior Information – Part II”</i>  Thomas Mejer Hansen, Knud Skou Cordua, Majken Caroline Looms, and Klaus Mosegaard (Computers & Geosciences, 52 (2013) 481-492)
<b>CERE 1316</b>	<i>“Improving Multi-point-based a Priori Models for Inverse Problems by Combining Sequential Simulation with the Frequency Matching Method”</i>  Knud S. Cordua, Thomas M. Hansen, Katrine Lange, Jan Frydendall, and Klaus Mosegaard (Presented at 82th Annual Meeting for the Society of Exploration Geophysicists (SEG 2012), Las Vegas, 2012)
<b>CERE 1317</b>	<i>“Multiple Scenario Inversion of Reflection Seismic Prestack Data”</i>  Thomas Mejer Hansen, Knud Skou Cordua, and Klaus Mosegaard (Presented at 74th EAGE Conference & Exhibition incorporation SPE EUROPEC 2012, Copenhagen, Denmark, 4-7 June, 2012)

<b>CERE 1318</b>	<i>“Heat of Absorption of CO2 in Aqueous Solutions of DEEA, MAPA and their Mixture”</i>  Muhammad Waseem Arshad, Nicolas von Solms, Kaj Thomsen, and Hallvard Fjøsne Svendsen (Energy Procedia, 37 (2013) 1532-1542) (Presented at the 11th International Conference on Greenhouse Gas Technologies (GHGT-11), Kyoto, Japan, 18-22 November, 2012)
<b>CERE 1319</b>	<i>“Freezing Point Depressions of Phase Change CO2 Solvents”</i>  Muhammad Waseem Arshad, Philip Loldrup Fosbøl, Nicolas von Solms, and Kaj Thomsen (Journal of Chemical & Engineering Data, 58 (2013) 1918-1926)
<b>CERE 1320</b>	<i>“Heat of Absorption of CO2 in Phase Change Solvents: DEEA and MAPA”</i>  Muhammad Waseem Arshad, Philip Loldrup Fosbøl, Nicolas von Solms, Hallvard Fjøsne Svendsen, and Kaj Thomsen (Journal of Chemical & Engineering Data, 58 (2013) 1974-1988)
<b>CERE 1321</b>	<i>“Binary and Ternary VLE of the 2-(diethylamino) -ethanol (DEEA)/3-(Methylamino)-propylamine (MAPA)/Water System”</i>  Ardi Harono, Fahad Saleem, Muhammad Waseem Arshad, Muhammad Usman, and Hallvard Fjøsne Svendsen (Chemical Engineering Science, 101 (2013) 401-411)
<b>CERE 1322</b>	<i>“Synthesis Methods in Phase Equilibria: Development and Testing of a New Apparatus”</i>  José M.S. Fonseca, and Nicolas von Solms (Accepted for publication in J. Supercritical Fluids)

<b>CERE 1323</b>	<i>“Inhibition of Gas Hydrate Nucleation and Growth: Efficacy of an Antifreeze Protein from the Longhorn Beetle Rhagium Mordax”</i>  Christine Malmos, Pei Cheng Chua, Nagu Daraboina, Dennis Friis, Erlend Kristiansen, Hans Ramløv, Malcolm A. Kelland, John Woodley, and Nicolas von Solms (Submitted for publication)
<b>CERE 1324</b>	<i>“Investigation of Kinetic Hydrate Inhibition using a High Pressure Micro Differential Scanning Calorimeter”</i>  Nagu Daraboina, Christine Malmos, and Nicolas von Solms (Energy & Fuels, 27 (2013) 5779-5786)
<b>CERE 1325</b>	<i>“Thermodynamic Promotion of Carbon Dioxide Clathrate Hydrate Formation – An Experimental Study”</i>  Peter Jørgensen Herslund, Kaj Thomsen, Jens Abildskov, Nicolas von Solms, Aurélie Galfré, Pedro Brântuas, Matthias Kwaterski, Jean-Michel Herri (International Journal of Greenhouse Gas Control, 17 (2013) 397-410)
<b>CERE 1326</b>	<i>“Application of the Cubic-Plus-Association (CPA) Equation of State to Model the Fluid Phase Behaviour of Binary Mixtures of Water and Tetrahydrofuran”</i>  Peter Jørgensen Herslund, Kaj Thomsen, Jens Abildskov, and Nicolas von Solms (Fluid Phase Equilibria, 356 (2013) 209-222)
<b>CERE 1327</b>	<i>”Simulations of Microbial Enhanced Oil Recovery: Adsorption and Filtration”</i>  Sidsel M. Nielsen, Igor Nesterov, and Alexander A. Shapiro (Accepted by Transport in Porous Media)

<b>CERE 1328</b>	<i>“Study of Wettability Alteration of the Oil-Brine System on Calcite Surfaces by enzymes”</i>  Alsu Khusainova, Sidsel Marie Nielsen, Hanne Høst Pedersen, John M. Woodley, and Alexander Shapiro (Submitted for publication)
<b>CERE 1329</b>	<i>“Prediction of Vapor-liquid Equilibria and Speed of Sound in Binary Systems of 1-alkanols and n-alkanes with the Simplified PC-SAFT Equation of State”</i>  Xiaodong Liang, Kaj Thomsen, Wei Yan, and Georgios M. Kontogeorgis (Fluid Phase Equilibria, 360 (2013) 222-232)
<b>CERE 1330</b>	<i>“Comparing the CAPCO2 Software to CASTOR pilot plant data Advanced thermodynamic models in rate based modeling”</i>  Philip Loldrup Fosbøl (Internal report)
<b>CERE 1331</b>	<i>“Experimental Determination and Modeling of the Phase Behaviour for the Direct Synthesis of Dimethyl Carbonate from Methanol and Carbon Dioxide”</i>  Ioannis Tsivintzelis, Nikolai E. Musko, Alfons Baiker, Jan-Dierk Grunwaldt, and Georgios M. Kontogeorgis (Journal of Supercritical Fluids, 84 (2013) 155-163)
<b>CERE 1332</b>	<i>“Poroelectricity of High Porosity Chalk under Depletion”</i>  Katrine Alling Andreassen, Ida Lykke Fabricius (Poromechanics V: Proceedings of the Fifth Biot Conference on Poromechanics, American Society of Civil Engineers, 2013, 2423-2430)

# Publications 2013

## New manuscripts

<b>CERE 1333</b>	<p><i>“Development and Analysis of the Original UNIFAC-CI Model for Prediction of Vapor-Liquid and Solid-Liquid Equilibria”</i></p> <p>Azizul Azri Bin Mustaffa, Rafiqul Gani, and Georgios M. Kontogeorgis (Accepted by Fluid Phase Equilibria)</p>
<b>CERE 1334</b>	<p><i>“A Comprehensive Framework for Surfactant Selection and Design for Emulsion Based Chemical Product Design”</i></p> <p>Michele Mattei, Georgios M. Kontogeorgis, and Rafiqul Gani (Accepted for publication)</p>
<b>CERE 1335</b>	<p><i>“The Role of Monomer Fraction Data in Association Theories – can we improve the Performance for Phase Equilibria Calculations?”</i></p> <p>Ioannis Tsivintzelis, David Bøgh, Eirini Karakatsani, and Georgios M. Kontogeorgis (Accepted by Fluid Phase Equilibria)</p>
<b>CERE 1336</b>	<p><i>“Negative Flash for Calculating the Intersecting Key Tie-lines in the MOC Solution of Gas Injection”</i></p> <p>Wei Yan, Michael L. Michelsen, and Erling H. Stenby (Presented at the IEA EOR 34th Annual Symposium, Stavanger, Norway, September, 2013)</p>
<b>CERE 1337</b>	<p><i>“Waterflooding Optimization in Uncertain Geological Scenarios”</i></p> <p>Andrea Capolei, Eka Suwartadi, Bjarne Foss, and John Bagterp Jørgensen (Published online)</p>

<b>CERE 1338</b>	<p><i>“On the Predictive Capabilities of CPA for Applications in the Chemical Industry”</i></p> <p>Ioannis Tsivintzelis, and Georgios M. Kontogeorgis (Submitted for publication)</p>
<b>CERE 1339</b>	<p><i>“Vapor-Liquid Equilibrium of Methane with Water and Methanol. Measurements and Modeling”</i></p> <p>Michael Frost, Eirini Karakatsani, Nicolas von Solms, Dominique Richon, and Georgios M. Kontogeorgis (Accepted by J. Chem. Eng. Data)</p>
<b>CERE 1340</b>	<p><i>“The Effect of Hot Water Injection on Sandstone Permeability”</i></p> <p>Esther Rosenbrand, Christian Haugwitz, Peter Sally Munch Jacobsen, Claus Kjøller, Ida Lykke Fabricius (Geothermics, 50 (2013) 155-166)</p>
<b>CERE 1341</b>	<p><i>“Rate and Predictors of the Conversion of Abstracts Presented at the Canadian Cardiovascular Congress Scientific Meetings to Full Peer-Reviewed Publications”</i></p> <p>W. Abuzeid, E. L. Fosbøl, P. L. Fosbøl, M. Fosbøl, S. Zarinehbab, H. Ross, D. T. Ko, M. C. Bennell, and H. C. Wijeysondera (Canadian Journal of Cardiology, 29 (2013) 1520-1523)</p>
<b>CERE 1342</b>	<p><i>“Improving GC-PPC-SAFT Equation of State for LLE of Hydrocarbons and Oxygenated Compounds with Water”</i></p> <p>Thanh-Binh Nguyen, Jean-Charles de Hemptinne, Benoit Creton, and Georgios M. Kontogeorgis (Submitted for publication)</p>

<b>CERE 1343</b>	<p><i>“On Solving the Rachford-Rice Equation with Higher Order Methods”</i></p> <p>Wei Yan, and Erling H. Stenby (Accepted by Fluid Phase Equilibria)</p>
<b>CERE 1344</b>	<p><i>“Design of an Emulsion Based Personal Detergent through a Model Based Chemical Product Design Methodology”</i></p> <p>M. Mattei, M. Hill, G.M. Kontogeorgios, R. Gani (Computer Aided Chemical Engineering, 32 (2013) 817-822)</p>
<b>CERE 1345</b>	<p><i>“Kaolinite Mobilisation in Sandstone: Pore Plugging vs Suspended Particles”</i></p> <p>Esther Rosenbrand, Ida Lykke Fabricius, Frans Kets (Proceedings, Thirty-Eighth Workshop on Geothermal Reservoir Engineering, Stanford University, Stanford, California)</p>
<b>CERE 1346</b>	<p><i>“Equivalent Pore Radius and Velocity of Elastic Waves in Shale. Skjold Flank-1 Well, Danish North Sea”</i></p> <p>Ernest N. Mbia, Ida L. Fabricius, and Collins O. Oji (Journal of Petroleum and Engineering, 109 (2013) 280-290)</p>
<b>CERE 1347</b>	<p><i>“Permeability, Compressibility and Porosity of Jurassic Shale from the Norwegian-Danish Basin”</i></p> <p>Ernest N. Mbia, Ida L. Fabrisius, Anette Krogsbøll, Peter Frykman, and Finn Dalhoff (Submitted for publication)</p>

<b>CERE 1348</b>	<p><i>“Caprock compressibility and Permeability and the Consequences for Pressure Development in CO<sub>2</sub> Storage Sites”</i></p> <p>Ernest N. Mbia (Accepted for publication)</p>
<b>CERE 1349</b>	<p><i>“Equilibrium Total Pressure and CO2 Solubility in Binary and Ternary Aqueous Solutions of 2-(Diethylamino)ethanol (DEEA) and 3-(Methylamino)propylamine (MAPA)”</i></p> <p>Muhammad W. Arshad, Hallvard F. Svendsen, Philip L. Fosbøl, Nicolas von Solms, and Kaj Thomsen (Accepted for publication)</p>
<b>CERE 1350</b>	<p><i>“Equilibrium Solubility of CO2 in Alkanolamines”</i></p> <p>Muhammad Waseem Arshad, Philip Loldrup Fosbøl, Nicolas von Solms, Hallvard Fjøsne Svendsen, and Kaj Thomsen (Presented at 7th Trondheim CCS Conference (TCCS-7), Trondheim, Norway, 4-6 June 2013) – Poster (Submitted for publication)</p>
<b>CERE 1351</b>	<p><i>“Fluid Phase Equilibria during Propylene Carbonate Synthesis from Propylene Oxide in Carbon Dioxide Medium”</i></p> <p>L. Gharnati, N. E. Musko, A. D. Jensen, G. M. Kontogeorgis, and J. D. Grunwaldt (J. Super. Fluids, 82 (2013) 106-115)</p>
<b>CERE 1352</b>	<p><i>“Association Theories for Complex Thermodynamics”</i></p> <p>G. M. Kontogeorgis (Chem. Eng. Res. Des. 91(10) (2013) 1840-1858)</p>

# Publications 2013

## New manuscripts

**CERE 1353**      “*Workshop on Industrial Use of Molecular Thermodynamics (InMoTher)*”

G. M. Kontogeorgis, J. N. Jaubert, J. C. Hemptinne (Oil & Gas Science and Technology-Revue d. IFP Energies Nouvelles, 68(2) 203-215)

**CERE 1354**      “*Development of a New Comprehensive Framework for Surfactant Selection and Design for Emulsion Based Chemical Product Design*”

Michele Mattei, Georgios M. Kontogeorgis, and Rafiqul Gani

(Presented at PPEPPD 2013, Iguazu Falls, Argentina-Brazil, 26-30 May, 2013)  
(Submitted for publication)

**CERE 1355**      “*Speeding Up Compositional Reservoir Simulation through an Efficient Implementation of Phase Equilibrium Calculation*”

Abdelkrim Belkadi, Wei Yan, Elsa Moggia, Michael L. Michelsen, Erling H. Stenby, Ivar Aavatsmark, Emanuele Vignati, and Alberto Cominelli (SPE 163589)(Presented at the SPE Reservoir Symposium, The Woodlands, Texas, USA, 18-20 February, 2013)

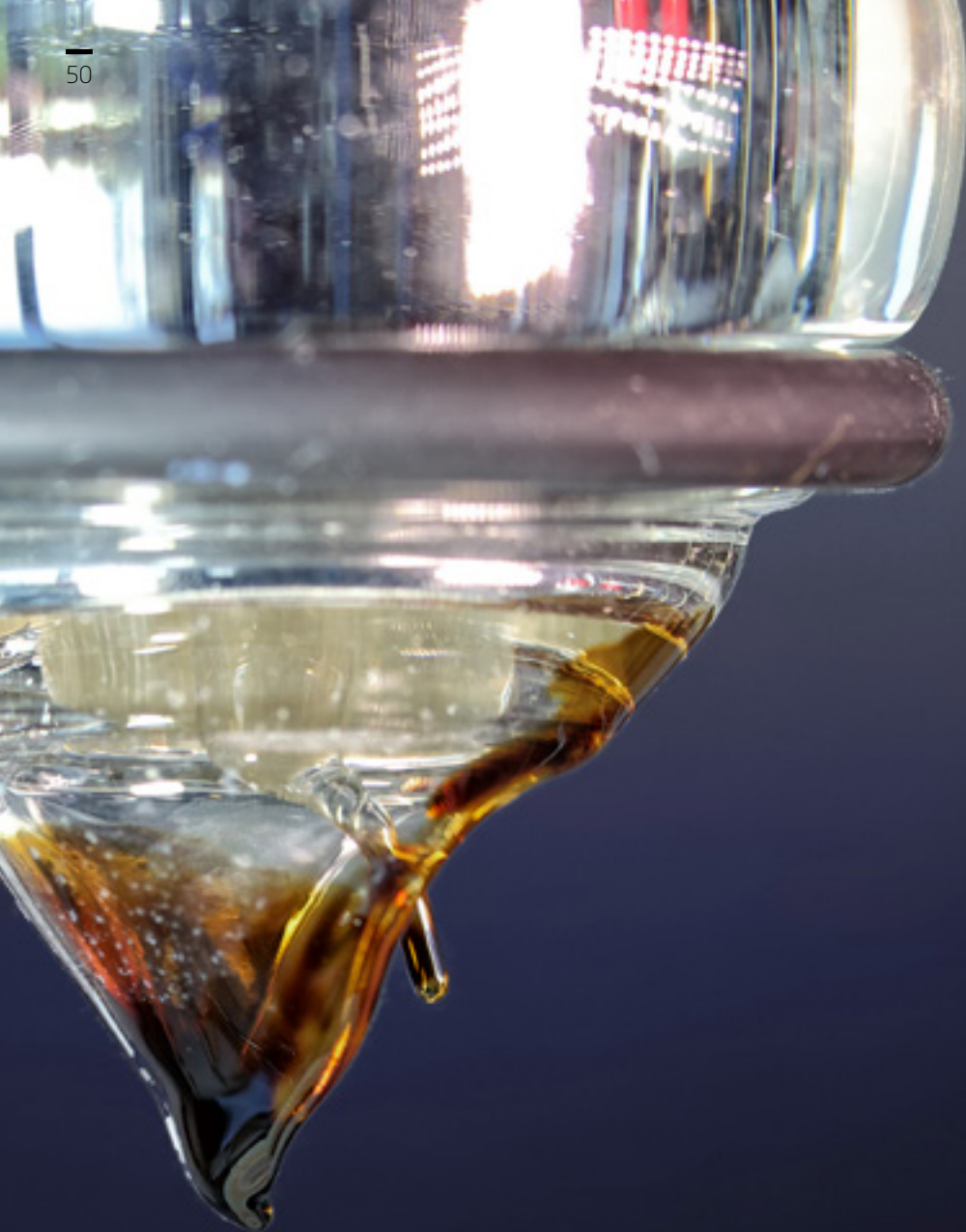
## Book Chapters

”Prediction of Thermo-physical Properties of Liquid Formulated Products”, M. Mattei, E. Conte, G. M. Kontogeorgis, and R. Gani

2013 Product Design and Engineering: Formulation of Gels and Pastes. Broeckel, V., Wagner, D. & Meier, W. (eds.). Wiley-VCH, 36 p.







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