## CERE ANNUAL REPORT 2015

### Electronic Version of the CERE Annual Report 2015

This printed report is a concentrated version of the CERE Annual Report 2015. The full report is found in a PDF version at CERE's website www.cere.dtu.dk

Besides carrying comprehensive versions of the articles, the e-report will have additional content which is not present in the printed report:

### Publications in 2015

CERE performs well in the world of energy resources engineering. This is reflected in the publications produced every year. The full list of 2015 publications is found in the e-report.

Conference Contributions & Invited Speakers The full list of conference contributions from CERE's researchers is found in the e-report.

### Master's Theses

The list of 2015 Master's Theses is found in the e-report.

CENTER FOR ENERGY RESOURCES ENGINEERING 00000

Technical University of Denmark





# 04

New Directions Following appointments of new faculty members and center coordinator, Chairman Georgios Kontogeorgis is looking forward to further discussions on the direction of CERE.

New People and

## The CERE Industrial Consortium

With three new members – MOL Group, Union Engineering and Calsep – CERE is now backed by more than 30 companies in its Industry Consortium.



### New Tools in Energy Resources Engineering

NMR scanning in reservoir geology and improved chemical engineering modeling tools for scaling, electrolytes, and deep oil exploration were presented at the CERE Discus-



Better Separation of Water from Natural Gas Multi-component potential adsorption theory (MPTA) is a valuable tool for improving the adsorption processes needed for separation of water

# 10

Simulations over Entire Oil Fields OPTION is a highly interdisciplinary Joint Industry Project which seeks to take oil production optimization to a new level



### News from CERE

Assistant Professor Katrine Alling Andreassen has been awarded the prestigious US Fulbright Visiting Scholars grant, and Dr. Bjørn Maribo-Mogensen (now with Linde, Germany) has been honoured by the European Federation of Chemical Engineering for his PhD at CERE.

### CERE Annual Report 2015

### Publisher

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**Cover photo** Oil drops on water



Will Future Oil Exploration be Airborne? Magnetic measurement techniques originally developed for space research seem promising for mapping the true extent of oil and gas



Precipitation helps Smart Water Flooding Surprisingly, precipitation during water flooding will not diminish, but rather increase oil production. This is one of the findings from a unique interdisciplinary four-year effort at



### Closing in on Shale and Heavy Oil Recovery

CERE has provided new reservoir simulation solutions for both production of liquid rich shale and production of heavy oil with a combination of steam and solvent.



### PhD Theses of the Year Main results from the PhD projects concluded during the year – five in all – are presented.

### New People and new Directions



Professor Georgios Kontogeorgis, Chairman of CERE gk@kt.dtu.dk Welcome! During 2015 CERE's structure has been consolidated with long awaited appointments of new faculty members from several departments; Xiaodong Liang as Assistant Professor at DTU Chemical Engineering, Arne Døssing Andreasen as Senior Researcher at DTU Space, and Associate Professor at DTU Compute Allan Peter Engsig-Karup joining CERE, while Philip Loldrup Fosbøl (DTU Chemical Engineering) was promoted to Associate Professor.

The new faculty members will further strengthen the center's activities in applied thermodynamics, scientific computing and geophysics. We should also mention that Dr. Hanne Pernille Andersen has been employed since May 2015 as Center Coordinator with special focus on future funding efforts and developing joint applications.

People are the most important asset of the center. We warmly welcome the new faculty members and center coordinator and the no less than six new PhD students and four post-doctoral researchers who joined CERE during 2015. We will make sure they feel comfortable and are well-integrated, and we are sure they will all contribute to the future development of CERE.

Last but certainly not least we would like to welcome three new member companies, Calsep, Union Engineering and MOL (the latter officially per 1.1.2016). We are confident that they will find their membership useful, and we hope that new projects will start with all of these companies in the near future.

### Time for strategy discussions

Now that the center's structure has been consolidated with the new faculty members and center coordinator, the time has come for further discussions during 2016 on potential focus areas and future perspectives of CERE. This will be a natural follow-up on the strategy process initiated after the international evaluation of the center in 2014.

One of the future perspectives will be our collaboration with the Danish Hydrocarbon Research and Technology Center (DHRTC). We expect that the first projects funded by DHRTC with CERE's participation will start during 2016. DTU has taken appropriate measures (see the News section for details) to ensure the synergy between CERE and DHRTC.

2015 was also the year when a number of large collaborative projects with participants from many CERE departments came to a conclusion. One of these projects, SmartWater, is about understanding the effect of water (with/without modifications) in enhanced oil recovery. This project is given extensive coverage in this year's report. Also featured are our Compplex, OPTION and MAPS projects. All of them are generously funded by companies – members of the CERE consortium – and some of them also by Danish Foundations and Councils.

#### Reasons to be proud

As always, the annual report highlights the PhD projects which have been completed. We thank the PhD students who have chosen to perform their projects at CERE, congratulate them on their achievements and wish all the best in their future endeavours. We expect to see several of them again in future collaborations. There are more reasons to be proud. Assistant Professor Katrine Alling Andreassen (DTU Civil Engineering) received the prestigious Fulbright visiting scholarship and she will spend 4 months in Colorado School of Mines during the first semester of 2016. Dr. Bjørn Maribo-Mogensen (DTU Chemical Engineering, now at Linde, Germany) received the excellence award for the best PhD thesis in thermo-dynamics from the European Federation of Chemical Engineering (Working Party of Thermodynamics and Transport Properties). More on these and other positive events is found in the News section.

### Busy conference organizers

In September 2015, CERE organized "Thermodynamics", a historical international conference in applied thermodynamics. The conference was held in Denmark for the first time and only 4th time outside UK in the conference's 24-year long history. The conference was a success with about 150 participants from 30 countries. In 2016, CERE will organize another well-known international conference, "Petrophase". This conference will be chaired by Associate Professor Nicolas von Solms and Senior Scientist Wei Yan. The "Petrophase" will take place at the Marienlyst Hotel in the city of Helsingør north of Copenhagen June 19-23, 2016 - just a few days after CERE's own Discussion Meeting at the same venue.

These conference activities put additional pressure on our already strained administrative personnel, so a special thanks from me for their continuous efforts, including the extra support during the busy 2015.

I hope you will enjoy the report. Should you have comments or questions after reading it, I will appreciate if you contact me. Feedback and suggestions are very important for our future development. We look forward to an equally exciting 2016 and I hope to see you at the annual CERE Discussion Meeting in June.

Professor Georgios Kontogeorgis, Chairman of CERE

## The CERE Industrial Consortium

CERE is supported by public means from several sources, e.g. The Danish Council for Independent Research - Technology and Production Sciences, EU framework programs for science and innovation, and The Danish Innovation Fund. Furthermore the center is supported by grants from several private companies.

The strongest asset of CERE is the Industry 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 our 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 ...

**MOL Group** is a leading integrated Central & East European oil and gas corporation headquartered in Budapest, Hungary. It has operations in over 40 countries and employs almost 30,000 people worldwide. MOL's exploration and production activities are supported by more than 75 years' experience in the hydrocarbon field. 36 million barrels of oil equivalent is produced annually, and reserves total 555 million barrels of oil equivalent.

**Union Engineering** is an engineering company specialized in sustainable technologies for capturing, recovering and purification of carbon dioxide. Main activities include engineering, procurement, construction, and maintenance of modular and individually designed CO<sub>2</sub> plants. With more than 1,000 CO<sub>2</sub> plants delivered throughout the last 30 years, installations in 110 countries and a wide range of patents, Union Engineering has become a leader in the industry.

**Calsep** stands for CALculation of SEParation processes. Calsep is a specialist company within oil and gas properties and phase equilibria. Consulting services and PVT and flow assurance software are the main products. Calsep has been a leading provider of PVT simulation services to the oil and gas industry for the last 30 years. Calsep offers PVT simulation studies within EOS Modeling and Flow Assurance for all kinds of fluids including natural gases, gas condensates, near critical fluids, black oils, and heavy oils.

AkzoNobel Research, The Netherlands BP Chemicals Limited, United Kingdom Calsep, Denmark Chevron, USA ConocoPhillips, USA DONG Energy, Denmark ENI S.p.A. Exploration and Production, Italy ExxonMobil Research and Engineering, USA Gassco AS, Norway Gassnova SF, Norway GDF SUEZ, France



- Hess Danmark ApS, Denmark IFP Nouvelles Energie, France Infochem Computer Services Ltd., United Kingdom Linde AG, Germany Lloyd's Register Consulting, Denmark Maersk Oil, Denmark
- MOL Group, Hungary
- National Oilwell Varco Denmark I/S, Denmark OMV E&P, Austria

RWE Dea, AG, Germany Schlumberger, USA Shell Global Solutions International B.V., The Netherlands SINOPEC, P.R. China SQM SA., Chile Statoil, Norway TOTAL, France Union Engineering, Denmark Welltec, Denmark

## New Tools in Energy Resources Engineering

While NMR scanning opens new frontiers for reservoir geologists, chemical engineers now have improved modeling tools for scaling, electrolytes, and deep oil exploration available.

In energy resources engineering, industry's desire to explore ever more complex natural conditions and develop advanced chemical engineering solutions goes hand in hand with academic aspirations. This was especially evident at CERE's Discussion Meeting, where members of the Industry Consortium met up with the scientific staff. The 2015 version of the annual event was well attended with 25 external participants representing 11 nationalities and 19 companies or external institutions.

Since the inclusion in 2009 of geological faculty, this field has grown steadily in CERE. At this years' Discussion Meeting both Professor Ida L. Fabricius, CERE, and Dr. Niels Christian Onno Van Gilse, DONG Energy, presented new petrophysical insight obtained through NMR (Nuclear Magnetic Resonance) scanning. While this method is still relatively new to oil and gas exploration, both presenters were confident that we will see a growing number of studies over the coming years.

As usual several sessions were devoted to new tools in chemical engineering. CERE has developed new software for simulations including scaling, electrolytes and refinements to thermodynamic models involving complex mixtures. Further, new tools for reservoir simulations and extensions of existing models to include HPHT (High Pressure, High Temperature) conditions were presented.

Shell "always sends new staff to Denmark" Stationed in the Netherlands Dr. Eric Hendriks heads the Process Simulation Thermodynamics team at Shell. "Our main job is to advice colleagues across the corporation on the use of physical property data. We always try to make people aware of limitations to the models. First of all the accuracy of the calculations will depend on the quality of the data fed into them."

Eric Hendriks' own background is in physics. He sees the Discussion Meeting as a fine venue for catching up on the latest developments in thermodynamic modelling.

"Take a model like the SAFT (Statistical Associating Fluid Theory, ed.). As a scientist I really like this model, even though I know it will be a no-go to use it in our own environment. Several fine academic careers can be attributed to some extent to SAFT, but I don't feel it is likely to conquer industry any day soon. A major problem in our context is the fact that various versions exist as individual scientists have shaped the model for their various purposes. Still, it is always interesting for us to come here and have a feel of what the most advanced academic simulation tools are capable of."

Shell has been a member of the Industry Consortium all along and frequently shares Master and PhD students with CERE.

"We attend the Discussion Meetings practically every year. And when we add new people to our team, my advice to them is always to go to Denmark."

### High validation demands from industry

Calsep provides software and consulting services within fluid modeling for clients in the oil and gas industry. The company has recently joined the CERE Industry Consortium. "Several of our employees have graduated from what is now CERE. We see CERE as having a good awareness of the practical aspects of their work. I see this as positive for our part. CERE is good at spotting trends in industry needs and converting this input into projects with useful applications", says R&D Manager Henrik Sørensen.

Currently the perspective of using CPA (Cubic Plus Association) as a supplement to the classical cubic equations of state has Calsep's particular focus. The CERE faculty have contributed strongly to the development of CPA.

"We see much interest in CPA from our clients, but for the oil industry there is a large step from showing interest in a new model to actually making use of it. Often our clients will prefer to live with the known uncertainty of a traditional



model rather than relying on a new and theoretically better model, which has not yet been thoroughly tested on the oil and gas application area. Our clients make huge investments based on the correctness of modeling results and they have very high validation demands. This is one of the fields where we contribute," says Henrik Sørensen.

### A national center for hydrocarbon research

A significant event since last years' Discussion Meeting was the inauguration of the Danish Hydrocarbon Research and Technology Center. Former CERE Chairman Erling H. Stenby presented the scope of the new institution in his capacity of scientific director for EOR activities.

Headquartered at DTU and collaborating closely with CERE, the national center has strong involvement from Maersk Oil and the other partners of the Danish Underground Consortium (DUC) both in terms of funding and joint projects. Still, Maersk Oil will continue its involvement in CERE activities, according to Dr. Niels Lindeloff, Lead Reservoir Engineer, Corporate Technology & Innovation:

"The two centers will have each their natural role. While the national center will always strive to push things towards implementation, CERE will be more academic. Once in a while you encounter problems so complex that you want to ask somebody with a narrow focus on exactly this issue. This may not happen often, but it is essential to know that when you are in this situation, you can find the right expert. This is one of the great strengths of CERE."

Another strong asset is the continuous success of CERE in attracting talents from

across the globe, Dr. Lindeloff notes: "As a Danish company we depend on a core of Danish employees to maintain continuity, but we are also highly dependent on international talent. If you want to recruit people with outstanding knowledge of a specific topic, obviously you cannot limit yourself to one nationality."

The CERE Discussion Meeting 2015 was held from June 17 – June 19 2015 at Comwell Borupgaard, Snekkersten. 25 external participants representing 11 nationalities and 19 companies or external institutions attended.

## Simulations over Entire Oil Fields

OPTION is a highly interdisciplinary Joint Industry Project which seeks to take oil production optimization to a new level.

The rate of production at one oil well may influence the expected output from another well in the same field either positively or negatively. It is therefore a natural ambition to simulate the production at all wells in the field in order to find the optimal way to produce the field. In other words, to find the solution that will result in the maximum output overall. This task is highly complex due to uncertainties in the geological data available. Further, it requires large computational resources as extremely large data sets are needed. The Joint Industry Project OPTION (Optimizing Oil Production by Novel Technology Integration) is set up to meet these challenges.

"We are confident that the project will result in unique software products and computational solutions which can be put to practical use through the industry partners. Key drivers of our efforts are efficient and robust mathematical algorithms combined with modern high-performance computing," says Allan P. Engsig-Karup, Associate Professor at DTU Compute and a new member of the CERE Faculty.

Not least the project partners Lloyd's Register Energy and Welltec are well suited for dissemination of resulting software and knowledge. Lloyd's Register Energy is a leading consultancy company to the energy sector, while Welltec develops and provides well technology and solutions for the oil and gas industry. Both companies were founding partners in OPTION in 2014. Since then DONG Energy has also joined.

"As scientists we are excited about the addition of DONG Energy to the project,

since this ensures our access to data from real oil production. This will provide a highly valuable verification of the simulations which we create," Allan P. Engsig-Karup notes.

### Strong synergy with industry

Allan P. Engsig-Karup joined the Faculty of CERE in 2015, following a DTU Compute colleague. Associate Professor John Bagterp Jørgensen became a CERE Faculty member two years earlier, and his early effort in the ADORE project contributed to lay the technology foundation for the OPTION project.

"John's work is close to the actual implementation of new solutions in optimization of oil production, while my own efforts are focused on core scientific computing components deep inside the software solutions, allowing us to make a difference as a team," explains Allan P. Engsig-Karup, noting that a range of other academic partners are also involved.

"The project is highly challenging, since we not only need to tackle the mathematical and computational challenges introduced by the various well locations and production rates, but also the large uncertainties related to the underground. While we may have some ideas about how the geology looks and which processes take place, we cannot know for sure. This complexity can only be addressed through a high degree of interdisciplinary cooperation. The combined knowhow from industry and academia has already proved a strong base for synergy within the project."

As a consequence of this cooperation, both Allan P. Engsig-Karup and Manager Stefan Glimberg of Lloyd's Register Consulting have recently completed an 11 month Executive MBA course at Harvard Business School. Entitled "Leading the Virtual Company" the course is highly relevant as the OPTION project spans across a range of groups and institutions. Faculty from DTU Mechanics, DTU Compute, DTU Chemistry, and the University of Copenhagen are involved.

### A new breed of scientists

The OPTION project has four PhD students and four Postdocs employed. Also, the project contributes in educating a significant number of Master and Bachelor students. Already in the first year, more than 20 people have been involved on the academic side of the project.

"An effort of this magnitude is close to being a guarantee for scientific progress. At the same time we contribute strongly to the training of a new breed of young scientists and engineers. Our ambition is to take the computational side of this field to a high international level, which has characterized the work of CERE's research within thermodynamic simulations and other traditional strongholds for the center."

Asked whether anything has surprised him in the project, he replies:

"I actually didn't expect it would be possible to mobilize so many people so quickly. The project has created a lot of possibilities. Especially for the students and young scientists we see a lot of doors opening. Besides the networking with other disciplines and with industry, they also get a feeling for other approaches, and how teaming up can overcome challenging problems. These experiences can surely be applied when new scientific challenges are encountered."

### The accuracy versus cost dilemma

A major challenge throughout the project is balancing the demand for accuracy with computational resources.

"We are always looking for smarter algorithms which will allow us to do calculations faster or with less computational costs. Still, we need to be careful not to simplify too much. To that



end we follow a dual approach. On the one hand we will do a full, expensive simulation and on the other hand we will experiment with new algorithms. We can then compare with the full simulation and evaluate if the faster and cheaper solutions are satisfactory."

The first application of OPTION software will probably be for optimization of production from an existing oil field. Further down the road Allan P. Engsig-Karup imagines that such software will be brought to use even before production starts:

"It is likely that we will actually be able to tell which combination of well sites will give the best overall production from the field."

The OPTION project was initiated in 2014 and is secured funding until autumn 2018.



Allan P. Ensig-Karup, Associate Professor



#### Data from the Danish oil field Stine, delivered by DONG, will be used to benchmark the reservoir simulation tool that applies the algorithms developed in OPTION.

### Lloyd's Register Consulting: Commercial Potential

Through the OPTION project Lloyd's Register Consulting has become a highly active member in the CERE Industry Consortium over a short time span. A joint Industrial PhD project within reservoir simulation led to the company's participation in the project.

"This OPTION project is now the largest R&D project for us in Denmark," notes Dr. Stefan Glimberg of Lloyd's Register Consulting

"Our own contribution will mainly be within the work packages on well flow and on the link between well flow and changes in the surrounding reservoir. This is predominantly where our expertise lies, and where we see the largest commercial potential as results will begin to emerge."

## **New Tools for** Shale and Heavy **Oil Recovery**



CERE has provided new reservoir simulation solutions for both production of liquid rich shale and production of heavy oil with a combination of steam and solvent.

The growing use of unconventional energy resource techniques presents reservoir simulations with severe challenges. A number of these are addressed in an ongoing Joint Industry Project at CERE named COMPPLEX (Compositional Reservoir Simulation Involving Complex Phase Equilibrium). The project mainly addresses production of liquid rich shale (LRS) and production of heavy oil using hybrid steam and solvent injection.

"We focus on the fundamental equilibrium description and calculation in those areas," says Senior Scientist Wei Yan, heading COMPPLEX. "It is beyond doubt that the solutions will also be useful for other applications."

For liquid rich shale, the effects on phase equilibrium of small pores in tight rock have been evaluated. PhD student Diego Sandoval has developed code that can

calculate the phase envelope in the presence of capillary pressures.

"The preliminary results indicate that the effect of capillary pressure is modest. This is in contrast to assumptions based on some field observations, which had indicated that the small pores can change phase equilibrium dramatically," explains Wei Yan.

### Hybrid method saves energy

Heavy oil production with hybrid steam and solvent injection has recently been introduced. The method involves a lower consumption of both energy and water in comparison to the dominant SAGD

(Steam Assisted Gravity Drainage) method. However, the new hybrid injection method results in complicated equilibrium between multiple hydrocarbon phases. In addition, the mutual solubility between water and other phases cannot be neglected at the high temperatures of steam injection.

PhD student Duncan Paterson compared various advanced Equation-of-State models for heavy oil / steam / solvent systems. He has shown that the PH flash framework (proposed by Professor Emeritus Michael Michelsen, CERE) can be extended to multiphase scenarios and successfully handle challenging cases such as narrow boiling problems.

"The developed algorithm provides an will be made."

The results will be presented at the 2016 improved oil recovery symposium of the Society of Petroleum Engineers (SPE).

### ExxonMobil and ConocoPhilips

While the COMPPLEX project has already yielded results within both of its main focus areas, the efforts have only just begun, Wei Yan underscores:

"Development of complex phase behavior will always be a long term effort. We have solved some problems, but keep finding new and interesting challenges."

For liquid rich shale, a major challenge is to understand the phase equilibrium in confinement down to nano scales, and to evaluate its influence on shale gas / oil production. Further, research on the effect of adsorption is being conducted.

"It is expected that capillarity and adsorption can change the phase behavior but the impact on liquid rich shale production is still unknown," Wei Yan remarks.

The industry partners in COMPPLEX are ExxonMobil and ConocoPhilips, and additional companies will be welcome.

"In this context I would like to stress that the scope of the project is not fixed to just liquid rich shale and heavy oil production. Similarly challenging phase equilibrium problems can be found in simulation of other processes. Just to give examples this could be in gas injection

efficient and reliable solution to the multiphase PH flash," Wei Yan comments. "In the future, the PH flash will be implemented in a simulator and more optimization on the algorithm efficiency in a simulation context or CO<sub>2</sub> sequestration. The scope of the project can be expanded provided that more companies join," says Wei Yan.

### Affordable computing

The project has a generally relevant perspective, the Senior Scientist notes:

"Oil and gas exploration under extreme conditions and the increasing utilization of unconventional resources does pose new challenges for compositional reservoir simulations. It needs to be evaluated whether advanced thermodynamic models in more complex forms are needed to address ever more complex phase behavior. This must be done with an eve to the costs of these calculations. Phase equilibrium calculation is already computationally heavy, and we need to find ways to apply advanced thermodynamic models in affordable ways."



Wei Yan, Senior Scientis



## Oil Exploration Inspired by Space Technology

Through a refinement of magnetic measurements developed for earth observation purposes, Senior Researcher Arne Døssing hopes to map the true extent of oil and gas fields. Finding oil or gas is always good news to the energy industry, but the next obvious questions are: how large is the field? And in which directions does it extend from the successful drilling? Traditionally, the answers have been sought through seismic measurements, i.e. controlled explosions trigger sound waves which travel the underground, and the reflected signals are analyzed for structural information. Geophysicist Arne Døssing, Senior Researcher at DTU Space and a new member of the CERE Faculty, proposes a different approach, namely to map the fields by airborne magnetic measurements.

"We cannot map the oil and gas directly, but it has been established that small amounts of gas leak from the fields to the geological layers above them. This will have spurred a change in the mineral composition in the above layers. It is the extent of this change, we may be able to map by magnetic measurements," explains Arne Døssing.

Magnetic measurements by earth observation satellites have become standard over the latest decades. These measurements serve various scientific purposes. Basically, the same technology can be used in oil and gas exploration but would need to be flown in aircrafts to get the necessary level of detail.

### Much cheaper than seismics

Magnetic measurements promise three large advantages compared with seismic measurements, Arne Døssing underlines:

"Firstly, the method would potentially save the companies large amounts of money. The equipment can be flown in small planes, and the whole operation would be much cheaper compared with seismic measurements. Secondly, the magnetic measurements are non-invasive and thus more environmentally benign. Thirdly, the magnetic signal is potentially a direct tracer of the hydrocarbons."

Why does the leakage of gas from deep oil and gas fields change the mineral composition in the above geological layers? The gas will serve as nutrition for certain types of microbes in the ground, which through their metabolism change the geochemical conditions for certain magnetic minerals, such as magnetite. Even though the amounts of gas are tiny – the phenomenon is normally referred to as micro-leakage – it will have a significant effect, because the process has been ongoing since the deep field was formed millions of years ago.

#### Industry data will be needed

Despite the potential advantages of the proposed method, Arne Døssing recognizes that it will not become available to industry overnight:

"We need an extensive research program to learn exactly which mineral compositions we should be looking for, and also to verify that what we are seeing the effect of is actually underlying oil and gas fields. For the latter purpose we will need data from industry, and obviously companies guard this type of data carefully. Therefore we will need initially to do research that supports the feasibility of the method. Once this is in place, we are confident that companies will take an interest in the method and hopefully trust us with their data for this purpose."

The group of Arne Døssing will collaborate with groups at the Imperial College and Oxford University, both UK, on the subject.

#### Also relevant to geothermal energy

Arne Døssing joined DTU in 2010 to contribute to the Danish Continental Shelf

Project, which is mainly focused on the North Atlantic and the Arctic Ocean. As part of this project, he has worked intensively with airborne gravity and magnetic data together with seismic data. Based on later Danish Research Councils grants, he has been able to expand his efforts into a broader paleo- and rock-magnetic context through the study of magnetism in old rocks.

In 2015 this led to his inclusion to the Faculty of CERE, continuing a trend of adding geological and geophysical competencies to the center.

"Much of my work is similar to the existing geophysical efforts at CERE in terms of the heavy data sets and scientific computing involved. Still, I hope to add new value due to the fact that gravity, magnetic and rockmagnetic data in combination with e.g. geochemical, petrophysical and seismic data have hardly been applied in an energy resources context previously."

Besides oil and gas exploration the spaceinspired methods are relevant to a number of other energy resources contexts, not least to geothermal applications.

### **Call for Industry Cooperation**

Public funding for validation of the suggested airborne oil exploration method has been applied for, but competition for these funds is fierce. CERE therefore encourages companies who would be interested in contributing to the project financially or with data to get in touch with Arne Døssing.



Arne Døssing Andreasen, Senior Researcher

## In the Eye of the Hurricane

Center Coordinator at CERE.

our industry Consortium, and also internal

The Center Coordinator plays a key role

and individuals.

with the right timing. Another task is to see





at CERE's annual Internal Meeting.

Hanne Pernille Andersen moderating the discussion

## **New Faculty Member** in Thermodynamics

of topics covered by the center.

Advanced thermodynamic models are the key interest of Xiaodong Liang, who joined the faculty of CERE as Assistant Professor by April 2015. He is engaged in the further development and application of models such as the Perturbed-Chain Statistical Associating Fluid Theory (PC-SAFT) and the Cubic Plus Association (CPA).

"One of my areas of focus is to extend these models to more accurately handle hydrogen bonds. Also, I am active in applications for inhomogeneous fluids, e.g. interfaces," Xiaodong Liang states.

Xiaodong Liang was employed as a PhD student and then a postdoc at CERE in August 2011 before joining the Faculty. He obtained his Master's degree in chemical engineering at the East China University of Science and Technology (ECUST). He then worked more than four years in the

process solution industry as a research and development engineer, where he had been developing and maintaining thermodynamic models for a large commercial process simulator.

"Software implementation is also an important aspect of my work, and I am confident that my previous industry experience can be very helpful when joint industry projects are in question, especially when the projects are related to process simulation and modeling for petroleum, chemical and polymer industries, and for possible simulator development," says Xiaodong Liang.



Xiaodong Liang, Assistant Professo

## **A Green Version** of Natural Gas

Newly appointed Associate Professor Philip L. Fosbøl works in a classic CERE field – thermodynamics – but with an eye to a range of new applications.

Natural gas is already in widespread use for domestic heating, but according to Philip L. Fosbøl we may see renewable gas replacing gas from underground reservoirs in the future.

"Many countries already produce biogas from agricultural waste products, organic household waste etc. For a number of reasons it would be desirable if this gas could be utilized continuously rather than needing storage. One possible solution would be transforming the gas into methane - or bio-methane if you will - of a quality similar to that of the natural gas presently used," explains Philip L. Fosbøl, who was appointed Associate Professor by March 2015.

Previous to his recent appointment, he has been with CERE in various positions all the way from his Master thesis in chemical engineering and his PhD thesis.

### New corrosion issues in shipping

The topic for Philip L. Fosbøl's PhD study was corrosion caused by carbon dioxide. This is still highly relevant:

"We are planning a series of activities related to corrosion. Besides CO2 we will include corrosion caused by HCl, SO<sub>2</sub>, SO<sub>3</sub>, H2SO4, and other substances. Especially, the sulphur containing substances have become problematic in shipping in recent years. Previously, commercial vehicles would always go close to full speed in order to get from A to B as fast as possible. Today we see many operators using the so called slow steaming in order to cut fuel costs and pollution. This has reintroduced a number of corrosive problems."

CERE has purchased new equipment for the upcoming studies on corrosion.

Given the subject of his PhD thesis it was only natural that Philip L. Fosbøl soon became active in a number of CERE projects on CO<sub>2</sub> capture and CO<sub>2</sub> transport for later storage. While political and industry interest in CO2 capture and storage (CCS) is currently low in Denmark, Philip L. Fosbøl and CERE remain involved in a number of European projects.

"The main problem in current CO2 capture techniques is the high energy consumption, which adds to costs and makes the concept less climate friendly. Several alternative solvents with much lower energy consumption have been suggested but unfortunately these processes are too slow for handling the large quantities of flue gas involved. Our approach is to speed up certain low-energy solvents by the use of enzymes."

#### Conversion of bio-gas

Currently, the CERE researchers are looking for other contexts than CCS to apply their expertise within the handling of CO2. "One idea is to capture CO2, not for storage, but for industrial use. This could be for sparkling beverages. Also a number of the techniques that we have applied in CO2 capture research have proven to be of general value. An example is how measuring speed-of-sound in a given media can reveal physical and chemical properties in a cost effective way."

Similarly, the basic thermodynamic modeling involved in energy optimization of CO2 capture is applicable to a range of emerging topics.





"One example is the new CERE-led project SYNFERON which is focused on converting the important intermediate product "syn-gas" - which can be produced from biological sources – into either methane or bio-fuels. Obviously a lot of chemistry is involved, but quite soon one will also need to take a number of process simulation issues into account. Just as for CO<sub>2</sub> capture the energy consumption involved in the various alternative processes will be a critical parameter."

This leads back to the idea of converting biogas directly into (bio-)methane for distribution in the existing network for natural gas for domestic heating and similar purposes.

"We are looking at a range of different renewable energy possibilities. It is likely that not just one solution will dominate. Quite possibly different solutions both in terms of intermediate products and the final gas and liquid products will be best in different scenarios. Also a balance between direct consumption and different types of energy storage will need to be found. I am confident that our experience in process simulation and energy optimization will prove highly useful for all these purposes."



Philip L. Fosbøl Associate Professor

## The Surprising Role of Precipitation

Contrary to general beliefs, precipitation during smart water flooding will not diminish, but rather increase oil production. This is one of the findings from a unique interdisciplinary four-year effort at CERE.

Legend has it that smart water flooding was invented by chance as engineers accidently injected sweet water instead of sea water and to their surprise saw more oil being produced. A link to the change in salinity was obvious, but despite decades of attempts by research groups in several countries a clear-cut understanding of the exact mechanism did not emerge. This inspired CERE and industry partners to commence the SmartWater project in 2011. Today, as the initial funding expires, the scientists involved are closing in on especially one plausible mechanism, while not ruling out that other mechanisms may contribute partially.

"Based on our own experiments combined with all public available experimental studies, we see a positive correlation between precipitation of solid from the injected brine and oil production," says Associate Professor Kaj Thomsen, heading one of the three work packages in SmartWater.

"This does not mean that precipitation is the sole explanation behind the effect of smart water flooding, but it is definitely something we should be looking into."

### A low risk attempt at extra oil

The term "smart water flooding" does not have a clear scientific definition. But basically the idea is to displace oil from a reservoir by water with specific and wellknown contents of the different salts rather than just the random brine available where production takes place.

"Smart water flooding is the first obvious choice when your standard water flooding doesn't produce extra oil anymore," says

Associate Professor Alexander Shapiro, heading another work package. "If you can achieve your results just by some modifications to the sea water, which you have so plentifully at hand, it will normally be much cheaper in comparison with other enhanced oil recovery methods. A further advantage is low risk. If you apply smart water flooding to a field that was about to become unproductive anyway the worst that could happen would be that you don't get more oil."

The original introduction of smart water techniques was in the Middle East, where injection of sweet water instead of the usual salty water proved to increase yields in sandstone reservoirs.

The SmartWater project has the Danish part of the North Sea as its focus. From the outset it was clear that just using sweet water instead of sea water would not be the solution, as the geology in the North Sea is very different from the Middle East.

### Samples from Maersk Oil and DONG

The North Sea oil reservoirs are located in either chalk or greensand. Samples of both types of rocks have been used in the flooding experiments, performed in advanced equipment which was developed for the purpose at CERE in collaboration with Geo (Danish Geotechnical Institute). Samples have been provided by SmartWater industry partners Maersk Oil and DONG Energy, while sample saturation has been carried out at GEUS (the Geological Survey of Denmark and Greenland). Funding has been provided by the industry partners and by The Danish Energy Agency.

Around half of the world's proven

hydrocarbon reserves are in carbonate rock.

North Sea chalks are carbonates composed

developed from the diagenesis of biogenic

pelagic calcareous ooze. The chalk has a

homogeneous pore structure with a high

specific surface area. Therefore the solid has

large exposure to the fluid - be it either oil

or water from water flooding.

of micrometer sized particles which are



Greensands are composed of a mixture of massive clastic quartz sand and porous sand size aggregates of green iron bearing clay. In the present study these grains are composed of chlorite. Greensand petroleum reservoirs can be found all over the world.

"The SmartWater project fits in nicely with the efforts here at CERE into understanding the geology of hydrocarbon reservoirs,"

coordinator.

When rock acts like a sponge As early as 2002 did Ida L. Fabricius and her group take an interest in the phenomena.

"The weakening role of water flooding to the geological structures came as a surprise to many, but to a geologist it is really not so strange. We all know that clay becomes soft when you make it wet, and the effect of water flooding to a carbonate or greensand reservoir is not necessarily that different."

In fact this effect is one of the proposed mechanisms for the enhanced oil recovery in smart water flooding: as the structure becomes softer it could act as a sponge, letting go of the contained oil due to the load of the overlaying layers.

"This could still be a possible mechanism. It is highly feasible that more than one mechanism is involved. Quite possibly the situation is complex in the sense that certain mechanisms enhance or dampen the effect of others," says Ida L. Fabricius. "We would of course very much like to know the exact mechanisms involved in order to propose the optimal way to modify the water for a given field. Once we understand the mechanism, we may be able to suggest other modifications like having specific ions in your water. In my view we still cannot pinpoint the exact mechanism behind the effect of smart water flooding. Instead I would rather say that we have mapped the solution space."

notes Professor Ida L. Fabricius, heading the third work package and overall SmartWater



Associate Professo



Associate Professor



Ida L. Fabricius Professor



Philin L. Foshøl Associate Professo

## **Smart flooding is** relevant in Denmark

A further major achievement from the project is the significant amount of new experimental data. The data is especially valuable as the majority of experiments are done with real North Sea core samples, rather than outcrop samples.

"Before SmartWater it was not clear whether such flooding techniques would be effective in a Danish context. The project has established that smart water flooding may have an effect both in greensand and in carbonate rock from the Danish part of the North Sea. Further, the experiments have been conducted under temperatures and pressures that are relevant to Danish reservoirs", says Ida L. Fabricius.

From the outset SmartWater was set up as highly interdisciplinary. Chaired by Professor Erling H. Stenby, Director at DTU Chemistry, the project involved faculty and technicians at mainly DTU Chemical Engineering and DTU Civil Engineering. One work package led by Ida L. Fabricius pursued possible rock mechanical mechanisms. A second package led by Alexander Shapiro looked at the dynamics of displacement of oil by smart water. And finally, the third work package led by Kaj Thomsen and Associate Professor Philip L. Fosbøl investigated chemical mechanisms related to the ion composition of the brine, precipitation etc.

Philip L. Fosbøl has led the development and implementation of the main experimental equipment for SmartWater, which is the flooding facility situated at DTU Chemical Engineering. The equipment is fully automated and can be programmed to alter a number of settings e.g. during night operation without staff being present.

### Methods are useful in oil-spill detection

The flooding experiments are used in projects under all three work packages. Whether you investigate rock mechanical, oil-water, or chemical mechanisms, you will need data from experiments.

"After many experiments, we still don't have the final answer as to why smart water flooding works," admits Alexander Shapiro. He supervises a PhD project by Artem Alexeev, who investigates the dynamics of possible oil-water interactions involved.

"Accepting that precipitation has a role in the smart water flooding effect, as demonstrated by Kaj Thomsen and Philip L. Fosbøl's group, the next obvious question is which mechanism is responsible," explains Shapiro. "Artem Alexeev investigates a hypothesis saying that the precipitation causes an oil-ganglia to unstuck from the pore walls and become mobile."

As the project is still ongoing it is too early to confirm or dismiss the hypothesis. In general, one should be careful to draw conclusions too soon, Alexander Shapiro underlines:

"We are talking about very complex phenomena. Many factors influence the results from the flooding, and it is difficult to exclude all other factors except the one you want to investigate. But the really good news is that we have acquired an internationally unique setup. During SmartWater we have developed several methods that certainly will prove valuable in other contexts. Just to give an example we needed to be able to trace tiny amounts of oil in large quantities of brine. This is also what you need to do when you are faced with e.g. the removal of oil spills at sea. Further, the interdisciplinary character of the project means that we are able to use a range of highly specialized equipment in conjunction, and to perform multidisciplinary analyses of the smart water mechanisms."

### New applications of NMR scanning

A strong asset is NMR (Nuclear Magnetic Resonance) equipment purchased for

SmartWater and installed at DTU Civil Engineering. The NMR technique enables the scientists to establish the pore size in a given sample and also to see how oil and water, respectively, are distributed inside.

The NMR scans are done in three steps: First with a fully brine-saturated core sample, and then when oil has been introduced at GEUS. so that the core contains both water and oil. Finally the samples are scanned when the flooding experiment with a typical duration of a few months has been completed.

"The NMR spectrum is very sensitive to chemical and physical changes in the pore space", explains Konstantina Katika, PhD student at DTU Civil Engineering. "For instance, it may happen that a sample suffers from inner structural changes which cause bypass problems that again may disturb results. We are able to see such changes in NMR. In this way we are able to verify whether the experiment was successful."

While NMR has been used in relation to oil and gas engineering previously, this has mainly been for porosity assessment, Konstantina Katika notes:

"We have demonstrated that NMR is relevant to a number of energy resources engineering challenges. For instance, we have been able to see the precipitation phenomena predicted by the group at DTU Chemical Engineering."

The positive effect of precipitation was demonstrated convincingly in a literature study by PhD student Krishna H. Chakravarty, supervised by Kaj Thomsen and Philip L. Fosbøl. The study draws upon results from 61 smart water flooding EOR studies reported in the literature.



flooding," says Kaj Thomsen.

in flooding water is able to substitute substitution frees calcium ions making them available for formation of calcium salts

production. So it is a delicate balance. Still, we can say that at the moderate levels of

### Formation of scales can be predicted

which were swept of their oil as normal water flooding commenced, are blocked, the water will be forced into the smaller

emulsion formation thereby dragging oil

Extended UNIQUAC model, developed by

"The model is able to predict the formation Philip L. Fosbøl. "In principle the software is available to our Consortium members. I to a user-friendly stage, but rather is an

Ready for application by industry

other salts or minerals. These not-too-costly solutions are the main focus in SmartWater,"

with the oil prize currently being low.

The researchers realize that the demand for smart water solutions may be small, given the









## **Better Separation of Water from Natural Gas**

Multi-component potential adsorption theory (MPTA) is a valuable tool for improving the adsorption processes needed for the separation of water from natural gas.

When just produced, natural gas will always contain a certain amount of water. Separation of water from gas is relevant not only to the quality of the gas, but also for the avoidance of corrosion in pipelines and of formation of gas hydrates.

Further, the separation processes have become more complex as modern energy resources engineering involves vast quantities of gas hydrate inhibitors and other chemicals. How will this affect the desired adsorption? Another aspect is the fact that a number of competing adsorption techniques exist. For instance, silica-gels and molecular sieves are emerging techniques besides the more traditional types of adsorbents. Statoil engages strongly in experimental studies that aim at clarifying these issues, but as experiments are expensive and time-consuming it is highly desirable to also do simulations which may predict the adsorption efficiency for a given scenario.

### Theory for adsorption is revisited

For that purpose, Statoil funded a oneand-a-half year project by Postdoc Igor Nesterov at CERE. Entitled "Multicomponent Adsorption of Polar Substances" the project has revisited the multi-component potential adsorption theory (MPTA) originally proposed by Alexander Shapiro and Erling H. Stenby. The theory describes adsorption as segregation of a mixture in the external potential field emitted by the adsorbent. Each component is affected by its own potential, adjusted on the basis of an individual adsorption isotherm. The interaction between the different components in the mixture is described by an equation of state for the bulk phase.

Soon after its introduction in 1998 it became clear, that MPTA was able to predict adsorption just as well as other methods and had the additional advantage of being applicable in a wider range of scenarios, for example to adsorption of supercritical fluids. However, for the current problems facing Statoil and other energy companies the question was whether the MPTA was able to cope with the complex mixtures involved?

"Description of adsorption of mixtures containing polar and associating compounds has been problematic so far for all adsorption models, including the MPTA. However, in his postdoc project Igor Nesterov has demonstrated that the MPTA is applicable for the task when combined with the Cubic Plus Association (CPA) equation of state. A trick was to take into consideration that the different substances may occupy different volumes inside a porous adsorbent" says Associate Professor Alexander Shapiro, who co-supervised the project with Professor Georgios Kontogeorgis.

### Complex mixtures can be handled

The CPA – suggested by Georgios Kontogeorgis in 1996 - is an engineering model for bulk phase equilibria that makes it possible to describe mixtures containing associating compounds. "The combination of the MPTA with CPA makes it possible to extend the MPTA to polar and associating mixtures," says Alexander Shapiro.

"It is found that the MPTA can be used for such systems if the components of the mixture are taken with individual adsorption capacities. The different substances may, simply, occupy the different "holes" inside the porous space, or get attached to the different points on the surfaces. The capacities may be determined experimentally, by adjustment of the potentials to the data on singlecomponent adsorption. A problem was to understand what then will happen to the mixtures of such substances.





Alexander Shapiro, Associate Professor





## **NEWS** from CERE

## Head of Center visits Brazil

Professor Georgios Kontogeorgis, CERE Chairman, visited Rio de Janeiro, Brazil, 25-28 February, to lecture at the Federal University of Rio and to attend the successful PhD defence of Leticia Cotia dos Santos. Professor Kontogeorgis had co-supervised her project entitled "Development of an Association Model for Calculation of Phase Equilibria of Complex Mixtures with Emphasis on Interest in Systems for Natural Gas Processing." Main supervisor was Professor Frederico Wanderley Tavares of the Federal University of Rio, while Professor Victor Rolando Ruiz Ahón was co-supervisor.

### **Project on Bio-fuel Conversion Initiated**

An international consortium of private companies and research institutions headed by CERE has set out to create a platform for converting biomass into high-value energy resources. The project is focused on "syn-gas" – a mixture of H<sub>2</sub>, CO and CO<sub>2</sub>. The technology for the production of syn-gas from agricultural waste products and similar types of biomass is already present, but syn-gas is an intermediate product of limited value on its own. The project SYNFERON (Optimised SYNgas FERmentatilON for biofuels production) aims to develop efficient ways to convert syn-gas to fluid biofuels. The project has a budget of 2.8 million Euro. Funding is provided by Innovation Fund Denmark. The project was initiated in July 2015.

### Modelling of Electrolytes yields Award



Dr. Bjørn Maribo-Mogensen has been honoured by the European Federation of Chemical Engineering (EFCE) for his PhD work on the modelling of electrolyte solutions.

"The Federation congratulates you on your excellent PhD thesis, for which you received the best evaluation results in terms of breadth and depth of the thesis, dissemination of knowledge, originality of the topic studied and of the methodology followed, innovation and industrial relevance, and scientific impact of the work," states the letter from EFCE, awarding Dr. Maribo-Mogensen the EFCE Excellence Award in Thermodynamics and Transport Properties 2015.

With the award followed a cash prize and an invitation to present the work at the ESAT conference in Athens, Greece, in June 2015.

### Prestigious Editorial Post

By April 2015, Professor Georgios Kontogeorgis joined the editorial team of "Fluid Phase Equilibria". The journal publishes high quality papers on experimental, theoretical and applied research related to equilibrium and transport properties of fluid and solid phases. For more information about the journal, please visit www.sciencedirect.com/science/journal/03783812

### **Next stop Colorado**

CERE Faculty member Assistant Professor Katrine Alling Andreassen has been awarded the prestigious Fulbright Visiting Scholars grant. The Fulbright Program is the flagship international educational exchange program sponsored by the US government.

Katrine Alling Andreassen will be working on the research project "Linking physical behaviour of sedimentary rocks – from loose to well-cemented materials" during her four month visit to the Colorado School of Mines.

"I am very much looking forward to the collaboration with Dr. Manika Prasad of the Petroleum Engineering Department at the Colorado School of Mines. She has an extensive knowledge within rock physics and geophysics and has worked with both elastic properties and acoustic properties of various rock types," says Dr. Andreassen.

The Fulbright Program awards approximately 800 grants to visiting scholars each year. Participants are chosen for their academic merit and leadership potential and are provided with the opportunity to conduct research and teaching in the US.

### **Thermodynamic Course Still going Strong**

CERE has a long history of hosting advanced courses on thermodynamic modelling for its own PhDs and industry. The 2015 version was entitled "Thermodynamic models – fundamentals and computational aspects" and took place on 10-21 August. The course was originally co-created by Professor Emeritus Michael L. Michelsen and Professor Jørgen Mollerup. Professor Michelsen has been teaching through all the years until recently, and he also participated this year in a consultancy capacity. The course was fully booked – also in accordance with tradition – and it was once again very well-received by the participants. CERE plans to run the course again in August 2016.



### **Petroleum Engineers of the Future**

It is a long tradition for DTU to once a year host one of the monthly meetings of the Society of Petroleum Engineers (SPE) Copenhagen. In past years CERE has organized these meetings. This year, the meeting was organized by CERE and the Danish Hydrocarbon Research and Technology Center (DHRTC) jointly.

The meeting, held on 6 October, also served as the year's major SPE and DTU joint event. These annual meetings serve as an opportunity for researchers to present recent developments to the petroleum industry.

The three main presentations were given by PhD students Alay Arya, Farhad Varzandeh, and Amalia Yunita Halim, all from CERE.

Another tradition at the annual event is a poster contest. DTU Chemical Engineering Master students Eirini Adamopoulou and Konstantinos Lymperis were awarded first and second place. Besides the honour they will both be able to participate in the annual SPE student conference "East meet West" in Krakow, Poland.

## **NEWS** from CERE

### Petrophase Conference Comes to Denmark

For a week in June 2016 Denmark will be the place to be for the petroleum industry and scientists. Held annually since 1999, the Petrophase conference is devoted to properties and chemistry of petroleum fluids and their effect on producing, processing, and refining in the upstream, midstream, and downstream industries. Traditionally, the conference alternates between America (either North or South America) and Europe. Once before, in 2000, the conference took place in Denmark. The conference will be chaired by Associate Professor Nicolas von Solms, CERE, and co-chaired by Senior Researcher Wei Yan, CERE, and Dr. Simon Andersen, Schlumberger. The Petrophase 2016 will be held at the Hotel Marienlyst in Helsingør 19-23 June 2016. For further information, please visit: http://petrophase2016.com



### Thermodynamics Conference held in Copenhagen



It was a first for Denmark, when CERE hosted the 24th Thermodynamics Conference 15-18 September 2015. The biennial international thermodynamics conferences were championed in the 1960s by Max McGlashan and Sir John Rowlinson, and initiated in 1964 by Harold Springall. Although the original emphasis of the science presented at the meetings was on experimental thermodynamics and thermochemistry, the Thermodynamic Conference Series (TCS) now has a wide remit encompassing broad areas of the discipline including experiment, theory, and molecular simulation. The conferences were held in the UK until 2005 when the conference took place in Portugal. In view of the success of the Portuguese conference it was decided to hold TCS meetings in both the UK and continental Europe from then on.

### **Presence at Danish-Israeli Oil Symposium**

Professors Ida L. Fabricius and Georgios Kontogeorgis participated in a Danish–Israeli Oil & Gas Symposium in conjunction with the Universal Oil & Gas Conference (UOG) 16-19 November. Both the symposium and the conference took place in Tel Aviv. A large delegation of Danish scientists active in oil and gas research attended. The symposium gave the CERE delegation the opportunity to discuss collaborations with both Israeli colleagues and other Danish institutions. Professor Kontogeorgis moderated the discussion of the symposium findings in a plenary session during the UOG conference

### **New PhD Projects**

Measuring and Modelling of Chemical Sulphur Corrosion Mechanisms in Marine Diesel Engines. PhD student: Henrik Lund Nielsen. Supervisor: Philip L. Fosbøl. Co-supervisors: Peter Glarborg, Søren Kiil, Kaj Thomsen.

### **Nonlinear Model Predictive Control for Oil Reservoirs.** PhD student: Tobias Kasper Skovborg Ritschel. Supervisors: John Bagterp Jørgensen and Andrea Capolei.

**Estimation of Matrix Flow Contribution in Naturally Fractured Carbonates.** PhD student: Justin Brand Ferrell. Supervisors: Alexander Shapiro and Wei Yan.

**Optimal Control of PDE Constrained Systems.** PhD student: Lasse Hjuler Christiansen. Supervisor: John Bagterp Jørgensen.

Application of an Association Equation of State in Compositional Reservoir Simulation. PhD student: Andre Vinhal. Supervisors: Georgios Kontogeorgis and Wei Yan.

Simulation and Optimization of Oil Reservoirs in the Danish North Sea. PhD student Steen Hørsholt. Supervisors: John Bagterp Jørgensen, Hamidreza Maghami Nick, Andrea Capolei.

### Synergy with Hydrocarbon Research Center

Associate Professor Nicolas von Solms, CERE, has been appointed "Local Focal Point" for DTU in relation to the recently established Danish Hydrocarbon Research and Technology Centre (DHRTC), headquartered at DTU. Von Solms will spend about half of his time over the coming two years on his role as DTU focal point for DHRTC.

As a further strengthening of the collaboration between the two research centers, Professor Georgios Kontogeorgis, CERE, has been appointed DTU representative to the scientific committee of DHRTC.

The first projects involving CERE faculty funded by DHRTC are expected to commence by the beginning of 2016.

### **Continuation of the CHIGP project**

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The oldest of the ongoing Joint Industry Projects at CERE, CHIGP (originally an acronym for Chemicals-in-Gas-Processing, but the scope has been broadened over the years), continues to produce new research and collaborations. The latest addition will be a new PhD project on "Thermodynamics of Petroleum Fluids relevant to Subsea Processing" to start in 2016. The project is funded by Statoil (Norway) and will be supervised by Associate Professor Nicolas von Solms and Professor Georgios Kontogeorgis. Other CHIGP projects which continue in 2016 focus on the further development of the CPA equation of state for asphaltenes (Alay Arya) and electrolytes (Anders Schlajker).

### **New Postdoc Projects**

### Development of a 3D Microbial Enhanced Oil

**Recovery Simulator.** Postdoc: Igor Nesterov. Supervisors: Sidsel Nielsen, Alexander Shapiro. The project is a part of the BioRec project. Funding: The Danish Advanced Technology Foundation.

Phase Equilibrium and Property Calculations for Oil-Gas Systems with Revision of Lumping and Delumping Techniques. Postdoc: Igor Nesterov. Supervisors: Erling H. Stenby, Wei Yan. The project is a part of the OPTION project. Funding: Innovation Fund Denmark.

Adsorption and Desorption of Crude Oil on Silica and CaCO<sub>3</sub> Surfaces. Postdoc: Xioayan Liu. Supervisor: Erling H. Stenby. The project is part of the BioRec project. Funding: Maersk Oil.

**Shale Gas, State of the Art.** Postdoc: Morten Kanne Sørensen. Supervisor: Ida L. Fabricius. Funding: the Danish Environmental Protection Agency.

Carbon Neutral Energy Productions by Hydrate Swapping. Postdoc: Liang Mu. Supervisor: Nicolas von Solms. Funding: H.C. Ørsted Postdoc Programme co-funded by Marie Curie Actions.

# PhD Defences

### Mixtures of Oil, Water, and Polar Chemicals

Michael Frost, PhD. Currently with Novozymes

Full title: "Measurement and Modelling of Phase Equilibrium of Oil - Water - Polar Chemicals".

Supervisors: Georgios Kontogeorgis, Nicolas von Solms.

The project was funded by Statoil.

Vast quantities of production chemicals are used in modern oil recovery. These include methanol and/or glycols injected into the natural gas well stream to prevent the formation of gas hydrates during transportation and further processing. The trend towards long distance multiphase flow pipelines increases the need for accurate calculations of mixtures containing water, an inhibitor, a gas phase, and a condensed phase. Due to a number of incidents where hydrate formation has taken place unexpectedly, considerable safety margins are often applied. However, excessive use of inhibitors does have both economic and environmental consequences. Thus it would be highly desirable if these processes and conditions could be predicted accurately. The project contributes to this end by a dual approach involving both phase behaviour modelling and experiments.

While several methods for prediction of phase behaviour in oil-water-inhibitor mixtures do exist, the results have so far been poor for high pressure systems (above 30 MPa), for systems with high concentrations of acid gas, and for estimating the partition of the inhibitor between the aqueous and the organic phases. Further, it is generally accepted that the field suffers from a lack of high-quality experimental data which are needed to verify the developed simulation tools.

The study focuses mainly on MEG (Monoethylene Glycol) and methanol, two of the most important hydrate inhibitors in use. A cornerstone of the project was the development and construction of a new VLLE (vapour-liquid-liquid-equilibrium) cell capable of reproducing the complex recovery conditions. Also an existing VLE (vapour-liquid-equlibrium) cell was used. Experimental studies of phase equilibrium were carried out for oil, MEG, and water systems at Statoil R&D, Norway. In the systems of oil + MEG, the mutual solubility increases with increasing temperature, with the solubility of aromatic hydrocarbons being higher than that of naphthenic and paraffinic hydrocarbons in each carbon fraction. Detailed investigation of hydrocarbon solubility in the polar phase





Schematic representation of the experimental set-up for the measurement of multiphase equilibria. – A: High pressure cell with 360° sapphire window. B: Temperature compensated high precision pressure sensor. C: Video camera. D: Platinum resistance thermometers Pt100. E: ROLSI<sup>™</sup> samplers. F: Cold light source with optical fibre. G: Remote control for the stirring motor. H: Low temperature chamber. I: Stirring motor. J: Data logger. K: Computer.

shows that benzene and toluene contribute a major part to the solubility of reservoir fluids in MEG. In the reservoir fluid + MEG + water system, the mutual solubility of MEG and oil decreases with increasing water content in the polar phase and the solubility of some hydrocarbon components become negligible. The data showed good reproducibility.

The experimental data were utilised for verification of VLLE predictions resulting from use of the CPA (Cubic Plus Association) equation of state with binary interaction parameters. The CPA was shown to be a powerful tool for predictions of mutual solubility in hydrocarbon systems containing water and gas hydrate inhibitors.

Finally, a comparison of CPA calculations was made between reservoir fluid and well-defined hydrocarbons in presence of polar chemicals such as water and MEG. Modelling results for reservoir fluid systems proved as good as for well-defined hydrocarbon systems.



- A. Equilibrium cell
- B. Pressure sensor
- C. Video camera
- D. Temperature sensors
- E. ROLSI<sup>TM</sup> samplers
- F. Cold light source
- G. Remote control for stirrer
- H. Temperature chamber
- I. Stirring motor
- J. Data logger
- K. Computer
- for data acquisition

### **Imaging of Oil** in Sea Water

### **Micro-organisms for Oil Recovery in Chalk**



"High-resolution

in Array Signal Processing"

Kim Knudsen. Funding The project was

jointly by the Danish National Advanced Technology Foundation. DTU Compute, and the Office of Naval Research.

Oil and gas exploration continues to move to greater depths. However, the environmental risk related to deep-water drilling was highlighted by the Deepwater Horizon oil spill in the Gulf of Mexico in 2010. The project addresses computational methods for detection and imaging of oil in the sea water column.

Previously, efforts for imaging of oil at sea have been focused at the surface. Remote sensing methods from satellites and aircrafts based on the interaction of electromagnetic waves with oil and water respectively are efficient for this purpose. However, far from all oil will reach the surface when a spill takes place at large depth. Much of the oil will be decomposed into stringy formations of viscous material mixed with water which remain trapped far below the surface.

Angeliki Xenaki, PhD. at DTU Elektro

Imaging Methods

Klaus Mosegaard,

funded

Traditional methods are inefficient for mapping submerged oil since electromagnetic waves attenuate fast when travelling in water. Instead, high-frequency acoustic methods are promising since they can overcome both the optical opacity of the water and resolve the small-scale structure of the new forms of oil.

Wide beam

transmitter

Schematic of a monostatic conguration for a multibeam echo sounder in the across-track plane.

The transmitter insonies the medium with a wide beam and beamforming attributes directivity

Transmi

Receive

to the receiving hydrophone array to localize the backscatterd returns.

Multichannel receiver

Sounder

Multibeam Echo

and beamforming

In the project, the submerged oil field is modeled as a fluid medium exhibiting spatial pertubations in the acoustic parameters from their mean ambient values which cause weak scattering of the incident acoustic energy. The study shows that highfrequency acoustic methods are suitable not only for large-scale localization of the oil contamination in the water column, but also for statistical characterization of the submerged oil field through inference of the spatial covariance of its acoustic parameters. Further, methods based on passive sonars were investigated. Conventional, beamforming acoustic methods suffer from resolution limitations related to the physical size and geometry of the array. Up-to-date methods for estimation of direction-ofarrival (DOA) involve a data cross-spectral matrix, which requires many snapshots - i.e. observation windows of the recorded wave-field - hence are suitable only for stationary incoherent sources. In this study, the DOA estimation problem is formulated both for single and multiple snapshots in the compressive sensing framework (CS). It is shown that CS has superior performance compared to traditional DOA estimation methods. This is especially true under challenging scenarios such as coherent arrivals, single-snapshot data and random array configurations. The high-resolution performance and the robustness of CS in DOA estimation are validated with experimental array data from ocean acoustic measurements.



Amalia Yunita Halim, PhD.

Currently Postdoc at the Research & Technology Center (DHRTC).

Full title: 'Application of Micro-organisms for Enhanced Oil Recovery".

Alexander Shapiro, Sidsel Marie Nielsen, Anna Eliasson Lantz.

The project was funded by Maersk Oil, DONG Energy, and The Danish Advanced Technology Foundation as a part of the BioRec project.

Microbial Enhanced Oil Recovery (MEOR) is an emerging technology. The project studies MEOR application in chalk reservoirs with special focus on petroleum reservoirs in the Danish sector of the North Sea. Although MEOR has been applied to a number of oil reservoirs worldwide, information on the application in chalk rock is scarce.

Initial investigations revealed spore-forming bacteria to be the most suitable for chalk. The spores are able to penetrate even in low permeable chalk and can survive periods of starvation. Among several bacteria studied, the spore-forming B. licheniformis 421 was selected as the model micro-organism.

When injected into homogeneous chalk cores after synthetic seawater flooding, the organism vielded 1.0 to 2.3 % additional original oil in place (OOIP) compared to baseline water flooding. Incremental recovery was significantly higher in heterogeneous chalk cores, where additional 6.9 to 8.8 % OOIP was recovered.

Investigations revealed selective plugging to be the main mechanism behind the increased level of production. During secondary oil recovery, when water is injected into an oil reservoir, the water tends to flow mainly through high-permeable channels. Thereby the water will bypass lowpermeable channels where oil is left. The selective plugging mechanism suggests that the injection of micro-organisms causes a blockage of the main channels, leading water to the previously bypassed pore spaces.

Further studies demonstrated that the bacteria were able to live in a high salinity environment. Anaerobic experiments showed that the bacteria were able to grow on different carbon compounds and to use nitrate as an electron acceptor. The bacteria preferred consuming n-alkanes instead of sugar compounds in molasses and produced a lipopetide biosurfactant, lichenysin G. The bacteria grew slowly when

> BACTERIA Cvanobacteria

The phylogenetic tree of life based on comparative ribosomal RNA homology. The tree shows the three domains of organisms and a few representative groups in each domain. All Bacteria and Archaea and most Eukarya are microscopic organisms. Animals, plants, and fungi are macroscopic Eukarya. LUCA, last universal common ancestor. Picture adapted from Madigan, M.T., J.M. Martinko, D.A. Stahl, and D.P. Clark, (2011). Ch 2. A Brief Journey to the Microbial World. In: Brock Biology of Microorganisms, 13th ed., Pearson Education, San Francisco, p. 36.

n-alkanes were present. However, significant formation of emulsion and reduction of interfacial tension (IFT) were still observed, even though hardly any bacterial growth occurred.

The project also studied stimulation of micro-organisms already present in a reservoir - indigenous microbes - as an alternative to injection of exogenous microbes. Anaerobic incubations using crude oil and brine from a North Sea reservoir showed that growth of indigenous microbes was stimulated by addition of molasses and by addition of nitrate. The growth of the indigenous microbes caused formation of emulsion and reduction of IFT in the crude oil-brine system.



### **Anti-freeze Proteins for Hydrate Inhibition**

### Improved Sonic Logs in Sandstone

### Perfeldt, PhD.

Full title<sup>.</sup> "Inhibition of Gas Hydrate Formation by Anti-freeze Proteins".

Supervisors: Nicolas von Solms, John M. Woodley.

Funding: The project was funded by DTU **Chemical Engineering**, Innovation Fund Denmark, Maersk Oil, DONG Energy, the **Danish Technological** Institute, and Roskilde University as part of the BioRec project.

Formation of gas hydrates is the leading flow assurance problem to the oil and gas industry. Traditionally, large amounts of thermodynamic inhibitors such as methanol and glycols have been used, but safety and environmental concerns have generated an interest in kinetic inhibitors, which show effect in much lower dosage. For instance water soluble polymers can be used to delay hydrate formation, but unfortunately these inhibitors have low biodegradability. The project investigates the effect of a proposed alternative type of environmentally benign kinetic inhibitors, namely anti-freeze proteins (AFP).

Several species of insects, fish and other animals produce anti-freeze proteins, which allow them to survive under cold conditions. In the project AFP I from the winter flounder and RmAFP1 from the beetle Rhagium mordax were investigated. Both were compared to two synthetic kinetic inhibitors, polyvinylpyrrolidone (PVP) and a modified polyvinylcaprolactam (LuvicapBio).

In a methane hydrate inhibition study using the Rocking cell, it was found that RmAFP1

### **Christine Malmos** Currently Postdoc at CERE.

had experienced nucleation before (memory solutions), RmAFP1 performed as effectively as PVP. RmAFP1 changed from promoting hydrate growth in fresh solutions to inhibiting growth in memory solutions. All the other kinetic inhibitors promoted growth in both fresh and memory solutions. In addition, a high pressure stirred cell (known as the Shell cell) was used to simulate more realistic conditions in presence of natural gas. Here, RmAFP1 inhibited hydrate nucleation significantly better than

LuvicapBio in both fresh and memory solutions. During hydrate growth, solutions with RmAFP1 formed slightly less hydrate in the fresh solution than the buffer. The results from these two studies suggest that RmAFP1 has a unique structure that could represent a new class of hydrate inhibitors.

clearly inhibited hydrate nucleation better

than PVP in fresh solutions. In solutions that

Further, the AFP I was studied in a saline solution with the presence of natural gas using the Rocking cell. Here, the kinetic hydrate inhibitors AFP I, PVP and LuvicapBio were found to inhibit hydrate nucleation similarly. However, AFP I inhibited the hydrate growth slightly better than the other KHIs. Dissociation of the hydrates showed that in presence of AFP I more stable hydrates were formed. In order to simulate a light liquid oil, n-heptane

was added to the saline solution. It was found that AFP I was inhibiting the hydrate nucleation, however less efficiently than PVP and LuvicapBio. In addition, solutions with AFP I and LuvicapBio were found to inhibit hydrate growth similarly, although PVP was the strongest growth inhibitor. However, hydrate dissociation showed that PVP stabilized the hydrates whereas in the presence of AFP I and LuvicapBio the hydrates were not stabilized and the dissociation profile was more simple. These results suggest that LuvicapBio and AFP I could be potential environmentally benign candidates for hydrate inhibition.

Finally, the influence of a hydrophobic surface on hydrate formation was studied in the presence of LuvicapBio and AFP I. Here, only very small amounts - around 0.02 wt% - of inhibitor were necessary in the hydrophobic coated crystallizer to achieve the same growth inhibition as with 0.2 wt% in stainless steel. Based on theoretical estimates of solid surface tension and work of adhesion, the following relationship was found: a lower solid surface tension meant less work of adhesion which resulted in less observed hydrate growth. The significant impact of the hydrophobic surface indicates that it could serve as a potential hydrate mitigation approach in the oil and gas industry.



Onset hydrate nucleation temperatures for the fresh solutions and memory solutions at a concentration of 2770 ppm. The lower onset temperature for the insect antifreeze protein RmAFP1 shows that it is an effective hydrate inhibitor and comparable with the commercial, non-biodegradable synthetic polymer PVP10.



### Morten Kanne Sørensen,

Engineering.

Full title: "Mud-filtrate Correction of Sonic Logs by Fluid Substitution.

Supervisor: Ida L. Fabricius.

The project was funded by DONG Energy.

Hydrocarbon exploration is pushed into unconventional reservoirs, often in complex geological structures. Making reliable discoveries in challenging conditions requires an increasing level in seismic interpretation. Contemporary techniques involve comparison with synthetic seismograms generated from velocity versus depth trends recorded as a sonic log in a borehole. However, shallow depth of penetration makes sonic logs sensitive to invasion of mud-filtrate from the borehole. The project uses a suite of experimental techniques in order to establish how this sensitivity can be adequately corrected for in sandstone.

Seismic exploration uses elastic waves to extract information about the subsurface. Application of advanced seismic interpretation requires ties between synthetic seismograms from sonic logs and seismic data. However, the constant over-pressure in the borehole relative to the formation pressure induces mud-filtrate invasion, which needs to be corrected for.

The volume of mud-filtrate to invade a formation is chiefly determined by the

properties of the mud. Minutes after the drill-bit penetrates a formation, filtration of solids at the borehole has formed a low permeable mud-cake. The pore-space of the formation determines how the invaded mud-filtrate is distributed. For sandstones of reservoir quality invasion affects the saturation deeper than the 20 cm which is probed by the sonic log.

Gassmann (1951) fluid substitution is a well-establish model for correction of sonic logs. However, the model is simplified in a number of ways, which makes a more accurate model desirable.

The project focuses on sandstone. The vast majority of sandstone reservoirs contain partial pore-filling clay, which was thus chosen as the main focus. Samples were thoroughly characterized by conventional core analysis, X-Ray Diffraction (XRD), Mercury Injection Carpillary Pressure (MICP), and low-field Nuclear Magnetic Resonance (NMR).



Radial saturation step profiles. In the case of WBM invading an hydrocarbon bearing zone (a) the saturation is reduced to the residual oil saturation, for OBM invasion the water saturation is reduced to the irreducible water saturation. For cases the saturation is mixed in the effective porosity and the irreducible water saturation remains saturated with the wetting fluid, which is water in this case.

Measurements of the elastic moduli as a function of water saturation during drying showed a distinct dependence of the characteristics of the pore-space, most notably the distribution of clay. Ultrasonic velocities in the fully saturated state were compared to those predicted by fluid substitution. The comparison showed heterogeneous pore-fill to cause a larger discrepancy than a uniform clay distribution. This departure is associated with fluid saturation retained in clay-filled pores. Incorporation of these pores in the solid framework composes an effective set of framework moduli applicable to a fluid substitution of the effective porosity only.

In conclusion, sonic log correction by fluid substitution reduces to an estimation of the distribution of clay. The critical evaluation is whether the clay distribution is heterogeneous. Distinction can be done by observation in the low-field NMR spectrum in the fully saturated state.

(a) WBM invading oil bearing sandstone







## Conference Contributions

#### JANUARY

4th International Workshop on Ionic Liquids Advanced Energy Applications WILS, Tarragona, Spain, 15-16 January 2015

F.M. Gaciño, T. Regueira, M.J. P. Comuñas, L. Lugo, and J. Fernández, "Isothermal compressibility of ionic liquids for their use as hydraulic fluids", 4th International Workshop on Ionic Liquids Advanced Energy Applications WILS, Tarragona, Spain, 15-16 January 2015 (oral)

#### FEBRUARY

### SPE Reservoir Simulation Symposium, Houston, Texas, USA, 23-25 February

Max la Cour Christensen, Umberto Villa, and Panayot Vassilevski, "Multilevel Techniques Lead to Accurate Numerical Upscaling and Scalable Robust Solvers for Simulation Symposium, Houston, Texas, USA, 23-25 February (oral)

Federal University of Rio de Janeiro, Brazil, 27 February, 2015

Georgios M. Kontogeorgis, "Equations of State in Three Centuries – What have we learnt? What more needs to be done?, Federal University of Rio de Janeiro, Brazil,

#### MARCH

SPE Forum Series, Physics and Chemistry in Nanoscale Rocks, La Jolla, California, USA, 22-26 March, 2015

Erling H. Stenby, "Thermodynamics in Confined Spaces and Modeling", SPE Forum Series, Physics and Chemistry in Nanoscale Rocks, La Jolla, California, USA, 22-26 March, 2015 (oral)

41st Conference on Phase Equilibria JEEP

T. Regueira, O. Fandiño, L. Lugo, E.R. López, and J. Fernández, "Phase behavior at high pressure of CO<sub>2</sub> + reference or vegetable lubricant systems developed for two stroke engines", 41st Conference on Phase Equilibria JEEP 2015, Coimbra, Portugal, 25-27 March 2015 (poster)

#### APRIL

### 3rd International Workshop on Rock Physics, Perth, Australia, 13-17 April, 2015

Konstantina Katika, and Ida Lykke Fabricius, "Electrical tortuosity, Kozeny's factor and cementation factor modelled for chalk", Proceedings of the 3rd International Workshop on Rock Physics, pages: 1-4, 2015, 3rd International Workshop on Rock Physics, 13-17 April, 2015, Perth, Australia (oral)

A. Awadalkarim, N.N. Foged, and I.L. Fabricius, "Elasticity and plasticity of Palaeogene clay from Fehmarn Belt area", 3rd International Workshop on Rock Physics, Perth, 13-17 April, 2015 (oral)

T.B. Gram, and I.L. Fabricius, "Water Weakening Effects: Elasticity of Reservoir Chalk with Partial Fluid Saturation", 3rd International Workshop on Rock Physics, Perth, 13-17 April, 2015 (oral)

M.K. Søerensen, and I.L. Fabricius, "Classification of sandstone by shale distribution and the effects on saturated elastic moduli", 3rd International Workshop on Rock Physics, Perth, 13-17 April, 2015

SPE Bergen One Day Seminar, Bergen, Norway, 22 April, 2015

D.C. Figueroa, P.L. Fosbøl, and K. Thomsen,

### 2015, Coimbra, Portugal, 25-27 March 2015

High Pressure High Temperature Fluids -Study on Black Oil", SPE Bergen One Day Seminar, Bergen, Norway, 22 April, 2015

K.H. Chakravarty, P.L. Fosbøl, and K. Thomsen, "Interactions of Fines with Oil and its Implication in Smart Water Flooding", SPE Bergen One Day Seminar, Bergen, Norway, 22 April, 2015 (oral)

### MAY

2nd IFAC Workshop on Automatic Control in Offshore Oil and Gas Production OOGP 2015, Florianópolis, Brazil, 27-29 May, 2015

A. Capolei, B. Foss, and J. B. Jørgensen, "Profit and Risk Measures in Oil Production Optimization", 2nd IFAC Workshop on Automatic Control in Offshore Oil and Gas Production OOGP 2015 Florianópolis, Brazil, 27–29 May 2015 (oral)

### CALPHAD XLIV meeting, Loano, Italy, *Mav 31 to June 5, 2015*

Kaj Thomsen "Modeling the solubility of ammonium and magnesium phosphates in multi-component solutions with the Extended UNIQUAC model", CALPHAD XLIV meeting, Loano, Italy, May 31 to June 5, 2015 (oral)

### JUNE

77th EAGE Conference & Symposium including SPE EUROPEC, Madrid, Spain, 1-4 June, 2015

K. H. Chakravarty, P.L. Fosbøl, and K. Thomsen, "Importance of Fines in Smart for Chalk Outcrops", 77th EAGE Conference & Symposium including SPE EUROPEC, Madrid, Spain, 1-4 June, 2015 (oral)

K.H. Chakravarty, P.L. Fosbøl, and K. Thomsen, "Interactions of Fines with Base Fractions of Oil and its Implication in Smart Water Flooding", 77th EAGE Conference & Symposium including SPE EUROPEC, Madrid, Spain, 1-4 June, 2015 (oral)

Konstantina Katika, Amalia Yunita Halim, Alexander Shapiro, and Ida Lykke Fabricius, "Quantification of the recovered oil and water fractions during water flooding laboratory experiments", Proceedings of the 77th EAGE Conference & Exhibition 2015, 2015, 77th EAGE Conference & Symposium including SPE EUROPEC, Madrid, Spain, 1-4 June, 2015 (oral)

I.L. Fabricius, E. Rosenbrand, Q. Fischer, and C. Grattoni, "Modelling Permeability in Rotliegend Gas Sandstones from NMR", Proceedings of the 77th EAGE Conference & Exhibition 2015, 2015, 77th EAGE Conference & Symposium including SPE EUROPEC, Madrid, Spain, 1-4 June, 2015 (oral)

International Symposium on Advanced Control of Chemical Processes, ADCHEM 2015, Whistler, British Columbia, Canada, 7-10 June, 2015

J. Gaspar, J.B. Bagterp, and P.L. Fosbøl, "Control of a post-combustion CO<sub>2</sub> capture plant during process start-up and load variations", International Symposium on Advanced Control of Chemical Processes, ADCHEM, Whistler, British Columbia, Canada, 7-10 June, 2015 (oral)

The Sixteenth International Conference on Petroleum Phase Behavior and Fouling, PetroPhase2015, Riviera Maya, México, 7-11 June 2015

Diego Sandoval, Wei Yan, Michael L. Michelsen, and Erling H. Stenby, "Calculation Of The Phase Envelope Change In Shale Due To Capillary Effects", The Sixteenth International Conference on Petroleum Phase Behavior and Fouling, PetroPhase2015, Riviera Maya, México, June 7-11, 2015 (oral)

Duncan Paterson, Wei Yan, Michael L. Michelsen, and Erling H. Stenby, "Phase Equilibrium Modeling of Heavy Oil/Steam/ Solvent Related Systems", The Sixteenth International Conference on Petroleum Phase Behavior and Fouling, PetroPhase2015, Riviera Maya, México, June 7-11, 2015 (poster)

Nicolas von Solms, "Gas hydrate formation and inhibition in the presence of crude oils" The Sixteenth International Conference on Petroleum Phase Behavior and Fouling, PetroPhase2015, Riviera Maya, México, 7-11 June 2015 (oral)

28th European Symposium on Applied Thermodynamics, ESAT 2015, Athens, Greece, 11-14 June 2015

T. Regueira, E.H. Stenby, and W. Yan, "Densities of the binary systems n-hexane + n-decane and n-hexane + n-hexadecane up to 60 MPa and 463 K", 28th European Symposium on Applied Thermodynamics, ESAT 2015, Athens, Greece, 11-14 June 2015 (oral)

Susana Almeida, Luis González Martos, Jordi Brull Costa, Rasmus Lundsgaard, Georgios M. Kontogeorgis, Jacob Sonne, Christian Wang, Adam Rubin, and Nicolas von Solms, "Predictive Modeling of Gas Diffusion and Solubility in Polymers for Offshore Application", 28th European Symposium on Applied Thermodynamics, ESAT 2015, Athens, Greece, 11-14 June 2015 (oral)

Fragkiskos Tzirakis, Paolo Stringari, Christophe Coquelet, Nicolas von Solms, and Georgios M. Kontogeorgis, "Hydrate equilibrium data for CO<sub>2</sub>+N<sub>2</sub> mixtures with TBAB, TBAF, CP, TBAB+CP, TBAF+CP promoters", 28th European Symposium on Applied Thermodynamics, ESAT 2015, Athens, Greece, 11-14 June, 2015 (oral) Alay Arya, Nicolas von Solm, and Georgios M. Kontogeorgis, "Modeling of Asphaltene System with the Cubic Plus Equation of State", 28th European Symposium on Applied Thermodynamics, ESAT 2015, Athens, Greece, 11-14 June, 2015 (poster)

Xiaodong Liang, and Georgios M. Kontogeorgis, "A new variant of the universal constants in the PC-SAFT EOS", 28th European Symposium on Applied Thermodynamics, ESAT 2015, Athens, Greece, 11-14 June, 2015 (oral)

Anders Schlaikjer, Kaj Thomsen, and Georgios M. Kontogeorgis, "Parameterization and Evaluation of the Electrolyte CPA Equation of State", 28th European Symposium on Applied Thermodynamics, ESAT 2015, Athens, Greece, 11-14 June 2015 (oral)

Georgios M. Kontogeorgis, "20 Years with the CPA Equation of State", 28th European Symposium on Applied Thermodynamics, ESAT 2015, Athens, Greece, 11-14 June 2015 (oral)

### 8th Trondheim Conference on CO<sub>2</sub> Capture, Transport and Storage, Trondheim, Norway, 16-18 June 2015

Arne Gladis, Maria T Gundersen, Philip Fosbøl, John M Woodley, and Nicolas von Solms, "Carbon dioxide absorption rate intensification by carbonic anhydrase for different solvent types", 8th Trondheim Conference on CO<sub>2</sub> Capture, Transport and Storage, TCCS 8, Trondheim, Norway, 16-18 June 2015 (poster)

D. Bonalumi, G. Valenti, S. Lillia, P.L. Fosbøl, and K. Thomsen, "A layout for the carbon capture with aqueous ammonia without salt precipitation", 8th Trondheim Conference on CO<sub>2</sub> Capture, Transport and Storage, Trondheim, Norway, 16-18 June 2015 (oral) J. Gaspar, A. Gladis, J.B. Bagterp, K. Thomsen, N. von Solms, and P.L. Fosbøl, "Dynamic Operation and Simulation of Post-Combustion CO<sub>2</sub> Capture," 8th Trondheim Conference on CO<sub>2</sub> Capture, Transport and Storage, Trondheim, Norway, 16-18 June 2015 (oral)

J. Gaspar, N. von Solms, K. Thomsen, and P.L. Fosbøl, "Multivariable optimization of piperazine CO<sub>2</sub> post-combustion capture process", 8th Trondheim Conference on CO<sub>2</sub> Capture, Transport and Storage, Trondheim, Norway, 16-18 June 2015 (oral)

Maria T Gundersen, Arne Gladis, Nicolas von Solms, and John M Woodley, "Reaction enhancement of post-combustion carbon capture using carbonic anhydrase", 8th Trondheim Conference on CO<sub>2</sub> Capture, Transport and Storage, Trondheim, Norway, 16-18 June 2015 (oral)

### 19th Symposium on Thermophysical Properties, Boulder, USA, 21-26 June, 2015

Susana Almeida, Luis González Martos, Jordi Brull Costa, Georgios M. Kontogeorgis, Jacob Sonne, Christian Wang, Adam Rubin, and Nicolas von Solms, "Predictive Modeling of Gas Diffusion and Solubility in Polymers for Offshore Application", 19th Symposium on Thermophysical Properties, Boulder, USA, 21-26 June 2015 (oral)

### IAS 31st Meeting of Sedimentology, Krakow,Poland 22-25 June 2015

L. Pasquinelli, I.L. Fabricius, N. Molenaar, J.S. Jeon, and S.R. Lee, "Thermal Properties of Gassum Fm and Recovery Efficiency for Thermal energy storage", IAS 31st Meeting of Sedimentology, Krakow, Poland 22-25 June 2015 (oral)

T.Orlander, L. Pasquinelli, and I.L. Fabricius, "Thermal conductivity of sedimentary rocks as function of Biot's coefficient". IAS 31st Meeting of Sedimentology, Krakow, Poland 22-25 June 2015 (oral)

ARMA 15-504 American Rock Mechanics Association The 49th US Rock Mechanics / Geomechanics Symposium, San Francisco, USA, 28 June-1 July 2015

K.A. Andreassen, and A. Al-Alwan "Rate Dependence of Dry, Oil- or Water-saturated Chalk", ARMA 15-504 American Rock Mechanics Association The 49th US Rock Mechanics / Geomechanics Symposium, San Francisco, USA, 28 June-1 July 2015 (oral)

SIAM Conference on Mathematical and Computational issues in the Geosciences, Stanford University, California, USA, June 29 - July 2, 2015

Max la Cour Christensen, "Element-Based Algebraic Multigrid Leads to Accurate Numerical Reservoir Simulation", SIAM Conference on Mathematical and Computational issues in the Geosciences, June 29 - July 2, 2015, Stanford University, California, USA (oral)

#### JULY

IAPWS symposium, Stockholm, Wednesday, 1 July 2015

Kaj Thomsen, and Muhammad Waseem Arshad, "Thermodynamic modeling of CO<sub>2</sub> capture system with liquid-liquid phase split in addition to VLE and SLE", IAPWS symposium, Stockholm, Wednesday, 1 July 2015 (oral)

13th International Conference on Carbon Dioxide Utilization, ICCDU, Singapore, Singapore, 5-9 July, 2015

Fragkiskos Tzirakis, Paolo Stringari, Christophe Coquelet, Nicolas von Solms, and Georgios M. Kontogeorgis, "Clathrate equilibrium data for CO<sub>2</sub>+N<sub>2</sub> mixtures with TBAB, TBAF, CP, TBAB+CP, TBAF+CP promoters", 13th International Conference on Carbon Dioxide Utilization, ICCDU, Singapore, Singapore, 5-9 July, 2015 (oral)

Nicolas von Solms, "CO<sub>2</sub> capture with gas hydrates", 13th International Conference on Carbon Dioxide Utilization, ICCDU, Singapore, Singapore, 5-9 July, 2015 (oral)

2015 CAS-TWAS Symposium on Green Technology for Sustainable Development, 2015 Green Tech, Beijing, China, July 23-25, 2015

Kaj Thomsen, "Phosphorus from Bio-waste, Thermodynamic Modeling", 2015 CAS-TWAS Symposium on Green Technology for Sustainable Development, 2015 Green Tech, Beijing, China, July 23-25, 2015 (oral)

2015 European Control Conference, Linz, Austria, 15-17 July, 2015

Jozsef Gaspar, John Bagterp Jørgensen, and Philip Loldrup Fosbøl, "A Dynamic Mathematical Model for Packed Columns in Carbon Capture Plants" (Proceedings from 2015 European Control Conference, (ECC), July 15-17, 2015, Linz, Austria) (oral)

### AUGUST

7th International Symposium on Molecular Thermodynamics and Molecular Simulation, Fukuoka, Japan, 4-7 August, 2015

Georgios M. Kontogeorgis, "Equations of State in Three Centuries – Perspectives and Future Challenges", 7th International Symposium on Molecular Thermodynamics and Molecular Simulation, Fukuoka, Japan, 4-7 August, 2015 (oral)

SPE Asia Pacific Enhanced Oil Recovery Conference, Kuala Lumpur, Malaysia, 11-13 August, 2015 K.H. Chakravarty, P.L. Fosbøl, and K. Thomsen, "Brine Crude Oil Interactions at the Oil-Water Interface", SPE Asia Pacific Lumpur, Malaysia, 11-13 August 2015 (oral)

### Joint Geothermal Seminar, Potsdam, Germany, 20 August, 2015

Tobias Orlander, "Poroelasticity and temperature of sedimentary rocks", Joint Geothermal Seminar, Potsdam, Germany, 20 August, 2015 (oral)

### SEPTEMBER

SPE Annual Caspian Technical Conference and Exhibition, Baku, Azerbaijan, 4-6 November 2015

K.H. Chakravarty, P.L. Fosbøl, and K. Thomsen, "Fine Formation During Brine-Crude Oil-Calcite Interaction in Smart Water Enhanced Oil Recovery for Caspian Carbonates", SPE Annual Caspian Technical Conference & Exhibition, Baku, Azerbaijan, 4-6 November 2015 (oral)

### IEA-EOR Workshop & Symposium, Sapporo, Japan, 7-11 September 2015

Amalia Yunita Halim, Sidsel Marie Nielsen, Anna Eliasson Lantz, Vural Sander Suicmez, Niels Lindeloff, Alexander Shapiro, and Erling Halfdan Stenby, "The potential of spore-forming bacteria flooding for enhanced oil recovery in a North Sea chalk reservoir", IEA-EOR Workshop & Symposium, Sapporo, Japan, 7-11 September 2015 (oral)

Diego Sandoval, Wei Yan, Michael L. Michelsen, and Erling H. Stenby, "Calculation of Multicomponent Phase Envelopes in the Presence of Capillary Pressure", IEA-EOR Workshop & Symposium, Sapporo, Japan, 7-11 September 2015 (oral)

Farhad Varzandeh, Wei Yan, Erling H. Calculation of HPHT Reservoir Fluids", IEA-EOR Workshop & Symposium, Sapporo, Japan, 7-11 September 2015 (oral)

A. Nermoen, R.I. Korsnes, I.L. Fabricius, and M.V. Madland, "Extending the effective stress relation to incorporate electrostatic effects", IEA-EOR Workshop & Symposium, Sapporo, Japan, 7-11 September 2015 (oral)

### 3rd Post Combustion Capture Conference, PCCC3, Regina, Canada, 8-11 September

Arne Gladis, Maria T. Gundersen, Philip L. Fosbøl, John Woodley, and Nicolas von Solms, "Kinetics of Carbonic Anhydrase in Promoted Chemical Solvents for Carbon Dioxide Absorption", 3rd Post Combustion Capture Conference, PCCC3, Regina, Canada, 08.09.2105. (oral)

Maria T Gundersen, Arne Gladis, Nicolas von Solms, and John M Woodley, "Technical anhydrase in post-combustion carbon capture", 3rd Post Combustion Capture Conference, PCCC3, Regina, Canada, 08.09.2105. (oral)

J. Gaspar, J.B. Jørgensen, L.R. Sandoval, "Controllability and Flexibility Analysis of a CO2 Capture Plant using MEA and Piperzine Promoted K<sub>2</sub>CO<sub>3</sub>", 3rd Post Combustion Capture Conference, PCCC3, Regina, Canada, 8-11 September 2015

H.L. Nielsen, J. Gaspar, and P.L. Fosbøl, "Rate-Based Modelling and Simulation of CO<sub>2</sub> Absorption and Desorption using Piperazine Promoted Potassium Carbonate", 3rd Post Combustion Capture Conference, PCCC3, Regina, Canada, 8-11 September 2015 (oral)

### Thermodynamics 2015, Copenhagen, Denmark, 15-18 September 2015

T. Regueira, E.H. Stenby, and W. Yan, "High pressure phase equilibrium measurement of methane + n-decane", Thermodynamics 2015, Copenhagen, Denmark, 15-18 September 2015, (poster)

Jordi Brull Costa, Rasmus Lundsgaard, Georgios M. Kontogeorgis, Jacob Sonne, Christian Wang, Adam Rubin, Nicolas von Solms, "Transport of Gases in Polymers for Offshore Applications", Thermodynamics 2015, Copenhagen, Denmark, 15-18 September 2015 (oral)

Martin G. Bjørner, and Georgios M. Kontogeorgis, "Evaluation of the quadrupolar CPA EoS for modeling multicomponent CO<sub>2</sub>-mixtures", Thermodynamics 2015, Copenhagen, Denmark, 15-18 September, 2015 (oral)

Farhad Varzandeh, Wei Yan, and Erling H. Stenby, "Comparison of GERG-2008 and Soave-BWR for modeling of natural gas Copenhagen, Denmark, 15-18 September, 2015 (Poster+5 minute presentation)

Anders Schlaikjer, Kaj Thomsen and Georgios M. Kontogeorgis, "Parameterization and Evaluation of the Electrolyte CPA Equation of State", Thermodynamics 2015, Copenhagen, Denmark, 15-18 September 2015 (Poster+5 minute presentation)

Duncan Paterson, Wei Yan, Erling H. Stenby, and Michael L. Michelsen, "Comparison of Mixing Rules for Asymmetric Systems and Water", Thermodynamics 2015, Copenhagen, Denmark, 15-18 September 2015, (oral)

Nicolas von Solms, "Modelling, Simulation Promotion in Gas Hydrate Processes",

Thermodynamics 2015, Copenhagen, September 2015 (oral)

Society of Petroleum Engineers (SPE) Annual Technical Conference and Exhibition, Houston, Texas, USA, 28–30 September 2015

D. Sandoval, W. Yan, M.L. Michelsen and E.H. Stenby, "Phase Envelope Calculations Capillary Pressure", Society of Petroleum Engineers (SPE) Annual Technical Conference and Exhibition. Houston, Texas, USA, 28–30 September 2015 (oral)

#### OCTOBER

### 85th Annual meeting of the SEG, New Orleans, 19-22 October 2015

A. Nermoen, R.I. Korsnes, I.L. Fabricius, and M.V. Madland, "Extending the effective stress relation to incorporate electrostatic effects", SEG Technical Program Expanded Abstracts 2015: 3239-3243, 85th Annual meeting of the SEG, New Orleans, 19-22 October 2015 (oral)

M.K. Soerensen, and I.L. Fabricius, "Fluid substitution in sandstone: Effective porosity or total porosity", Proceedings of the: 85th Annual meeting of the SEG, New Orleans, Oct. 19-22, 2015. SEG Technical Program Expanded Abstracts 2015: 3020-3024, 85th Annual meeting of the SEG, New Orleans, 19-22 October 2015 (oral)

M.K. Soerensen, and I.L. Fabricius, "Effect of brine saturation on the elastic moduli of compacted clay", Proceedings of the: 85th Annual meeting of the SEG, New Orleans, Oct. 19-22, 2015. SEG Technical Program Expanded Abstracts 2015: 3186-3190, 85th Annual meeting of the SEG, New Orleans, 19-22 October 2015 (oral)

#### NOVEMBER

SPE Caspian Technical Conference and Exhibition, Azerbaijan, 4-6 November 2015

K.H. Chakravarty, P.L. Fosbøl, and K. Thomsen, "Fine Formation During Brine-Crude Oil-Calcite Interaction in Smart Water Enhanced Oil Recovery for Caspian Carbonates", SPE Annual Caspian Technical Conference & Exhibition, Baku, Azerbaijan, 4-6 November 2015 (oral)

Abu Dhabi International Petroleum Exhibition and Conference. Society of Petroleum Engineers, Abu Dhabi, UAE, 9-11 November 2015

K.H. Chakravarty, P.L. Fosbøl, and K. Thomsen, "Significance of Fines and their Correlation to Reported Oil Recovery", Abu Dhabi International Petroleum Exhibition and Conference, Society of Petroleum Engineers, Abu Dhabi, UAE, 9-11 November 2015 (oral)

SPE OGICE 2015, Mumbai, India 24-26 November 2015

K.H. Chakravarty, P.L. Fosbøl, and K. Thomsen, "Formation of Anhydrite Due to Interaction Between Water Soluble CO2 (aq) and Calcite Mineral During Enhanced Oil Recovery", SPE Oil & Gas India Conference and Exhibition, Mumbai, India 24-26 November 2015 (oral)

EGATEC 2015, Vienna, Austria, 25-26 November 2015

Farhad Varzandeh, Wei Yan, and Erling H. Stenby, "Comparison of GERG-2008 and Soave-BWR in PVT Modeling and Thermal Properties Calculation of Natural Gas Systems", EGATEC 2015, Vienna, Austria, 25-26 November 2015 (Oral)



MASTER THESES



lens Hedegaard

**Bjørn Harald Høgmo** 

and conceptual well design"

"Simulation of Oil Reservoirs"

Peter Sally Munch Jacobsen

"Geochemical Modelling of Heat

Steen Hørsholt

Treated Sandstone"

"Dispersion of elastic waves in shale"

"Challenges and techniques related to

drilling through carbonate formations

### Master Theses 2015

Peter Edward Ackermann "Stochastic Optimization and Risk Management in the Production Optimization of Oil Reservoirs"

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Mamuna Afzal "Experimental study of enzyme applicatbility for enhanced oil recovery"

Mehrdad Akhami "Smart waterflooding of petroleum reservoirs: verifying the models with experimental data"

**Firas Al-Matook** "Important Concepts within Oil Well Drilling Procedures"

Aleksander F. Amundsen

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membranes"

Jakub Benicek

"MEOR: Modellering and Numerical

Thorvaldur Tolli Ásgeirsson

"Modeling gas separation in polymer

"Application of emulsion-forming enzymes

Julie Pauline Flensborg "Phase transition analysis and optimization of natural gas using equation of states"

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with CFD Tools"

**Mindaugas Genys** 

nanotechnology"

**Morten Hansen** 

"Wettability alteration using

"Density and viscosity of hydrocarbon

mixtures at high pressures and high

Lasse Hjuler Christiansen

Optimization for Oil Reservoir

**Hilmar Mar Einarsson** 

"Multi Objective PDE Constrained

"Simulation of Reservoir Processes

**Mik Fournais** "Influence by Porefluid on Rate-dependent Deformation of Chalk"

Tomasz Krzysztof Jacyno "Permeability and elasticity of Polish Palaeozoic shale"

> Claus Lenander Jensen "Reduced Order Modelling for Partial Differential Equations"

**Morten Walk Jensen** "Pilot scale experimental studies and simulation of dynamic mode CO2 capture"

**Christian Frausing Brams** 

for enhanced oil recovery"

"A study on multiscale techniques for reservoir simulation"

**Tobias Anker Hansen** "Development of a predictive version of the CPA equation of state for applications in the chemical industry"

"Phase transition analysis and optimization

of natural gas using equation of states"

**Daniel Jonas** "Combined interpretation of NMR Core and Logging data"

**Dimitrios Kourmpetis** "Computer Modeling of Microbial Enhanced Oil Recovery"

Lasse Flindt Kristiansen "Geomechanical modelling of Shale overburden in the Danish North Sea"

Pernille Birkelund Larsen "Rock physical models of elastic wave data for palæozoic shale"

Alexander Oduro "Log interpretation of Harald Field"

**Christian Hjort Larsen** "Drilling through shaly overburden"

**Antonios Pantelak** "Phase behavior study of hydrocarbon mixtures with an HPHT PVT apparatus"

Nicolai Lindskov "Polyaxial strength criteria applied in tunneling"

**Georgia Pantelide** "Phase behavior study of hydrocarbon mixtures with an HPHT PVT apparatus"

Anders Lodberg "Modeling and experiments for recycling of phosphorus"

**Christian Wichmann Moesgaard** 

"Massively parallel nonlinear multigrid

"Simulation of heat pump for flue gas

on modern architectures"

Mohamud Abdi Muse

from wood chip combustion"

Management"

"Design of process for the removal of SO2 from diesel exhaust"

Amir Hossein Shamsolhodaei "Strength criteria from rock mechanical tests"



Randi Neerup "Kinetics of enzyme-enhanced CO <sub>2</sub> capture"	<b>Athanasios Stefanakis</b> "PVT in Shale Gas Production: Modelling and Simulation"
Henrik Lund Nielsen "Model development of rate based CO <sub>2</sub> capture columns with solid precipitating solvents"	<b>Unnur Margrét unnarsdóttir</b> "Methane production and CO <sub>2</sub> storage with hydrate swapping"
<b>Alexander Oduro</b>	<b>Vasos Vasou</b>
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Harald Field"	high pressures"
Antonios Pantelakis	Vegard Eriksen Aarsheim
"Deas behavior tudu of budus autom	"The Effect of Anti-Acolomousto on

The Effect of Anti-Agglomerants on Hydrate Formation in Real Systems"

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### **Tobias Kasper Skovborg Ritschel**

"High-Performance Computing for PDE Constrained Optimization in Oil Reservoirs

### Abduallah Mohammad Sayed

## **Publications**



### **Previously Submitted Publications**

CERE 1328	"Study of Wettability of Calcite Surfaces using Oil-Brine-Enzyme Systems for Enhanced Oil Recovery Applications"	CERE 1422	"New Variant of the Universal Constants in the Perturbed Chain-Statistical Association Fluid Theory Equation of State"	CERE 1430	"Modeling MEA with the CPA Equation of State: A Parameter Estimation Study Adding Local Search to PSO Algorithm"
	Alsu Khusainova, Sidsel Marie Nielsen, Hanne Høst Pedersen, John M. Woodley, and Alexander Shapiro (Journal of Petroleum Science and Engineering, 127 (2015) 53-64)		Xiaodong Liang, and Georgios M. Kontogeorgis (Industrial & Engineering Chemistry Research, 54(4) (2015) 1373-1384)		Leticia Cotia dos Santos, Frederico Wanderley Tavares, Victor Rolando Ruiz Ahón, and Georgios M. Kontogeorgis (Fluid Phase Equilibria, 400 (2015) 76-86)
CERE 1411	"Different Effects of Temperature and Salinity on Permeability Reduction by Fines Migration in Berea Sandstone"	CERE 1424	"Modeling Water Saturation Points in Natural Gas Streams Containing $CO_2$ and $H_2S$ – Comparisons with different Equations of State"	CERE 1431	"Thermodynamic Modeling of CO2 Absorption in Aqueous N-Methyldiethanolamine using Extended UNIQUAC Model"
	Esther Rosenbrand, Claus Kjøller, Jacob Fabricius Riis, Frans Kets, and Ida Lykke Fabricius (Geothermics, 53 (2015) 225-235)		Letícia C. dos Santos, Samir S. Abunahman, Frederico W. Tavares, Victor R. R. Ahón, and Georgios M. Kontogeorgis (Industrial & Engineering Chemistry Research, 54(2) (2015) 743-757)		Negar Sadegh, Erling H. Stenby, and Kaj Thomsen (Fuel, 144 (2015) 295-306)
CERE 1417	"Experimental Validation of Kinetic Inhibitor Strength on Natural Gas Hydrate Nucleation"	CERE 1425	"Two-Phase Immiscible Flows in Porous Media: The Mesocopic Maxwell-Stefan Approach"	CERE 1432	"Testing Antifreeze Protein from the Longhorn Beetle Rhagium Mordax as Kinetic Gas Hydrate Inhibitor using a High Pressure Micro Differential
	Nagu Daraboina, Stylianos Pachitsas, and Nicolas von Solms (Fuel, 139 (2015) 554-560)		Alexander A. Snapiro (Transport in Porous Media, 107(2) (2015) 335-363)		Scanning Calorimeter Nagu Daraboina, Christine Malmos, and Nicolas von Solms (Can. J. Chem., 93 (2015) 1025-1030)
CERE 1418	<i>"The Combined Effect of Thermodynamic Promoters Tetrahydrofuran and Cyclopentane on the Kinetics of Flue Gas Hydrate Formation"</i>	CERE 1426	"Modeling of Dissolution Effects on Waterflooding"	CERE 1433	"Natural Gas Hydrate Formation and Inhibition in Gas/Crude Oil/Aqueous Systems"
	Nagu Daraboina, and Nicolas von Solms (J. Chem. Eng. Data, 60 (2015) 247-251)		Artem Alexeev, Alexander Shapiro, and Kaj Thomsen ( <b>Transport in Porous Media,</b> 106(3) (2015) 545-562)		Nagu Daraboina, Stylianos Pachitsas, and Nicolas von Solms (F <b>uel, 148 (2015) 186-190)</b>





### New Manuscripts 2015

CERE 1501	"PVT Modeling of Reservoir Fluids using PC- SAFT EoS and Soave-BWR EoS" Wei Yan, Farhad Varzandeh, and Erling H. Stenby (Fluid Phase Equilibria, 386 (2015) 96-124)	CERE 1505	"Short Communication. A Comment on Water's Structure using Monomer Fraction Data and Theories" Xiaodong Liang, Bjørn Maribo-Mogensen, Ioannis Tsivintzelis, and Georgios M. Kontogeorgis (Submitted for publication)	CERE 1509	"Solubility of Hydrogen Sulfide in Aqueous Solutions of N-Methyldiethanolamine at High Pressures" Negar Sadegh, Kaj Thomsen, Even Solbraa, Eivind Johannessen, Gunn I Rudolfsen, and Ole J. Berg (Fluid Phase Equilibria, 393 (2015) 33-39)
CERE 1502	"Multicomponent Adsorption Model for Polar and Associating Mixtures" Igor Nesterov, Alexander Shapiro, and Georgios M. Kontogeorgis (Ind. Eng. Chem. Res., 54 (2015) 3039-3050)	CERE 1506	"Vapor Liquid Equilibrium Measurements and Modeling of 1-propanethiol + 1-butanethiol + CH4 Ternary System at 303, 335 and 368 K with a Pressure Variation from 1 to 9 MPa" Javeed A. Awan, Ioannis Tsivintzelis, Christophe Coquelet, and Georgios M. Kontogeorgis (Submitted for publication)	CERE 1510	"Modeling Phase Equilibria for Acid Gas Mixtures using the CPA Equation of State. Part VI. Multicomponent Mixtures with Glycols Relevant to Oil & Gas and Liquid or Supercritical CO2 Transport Applications" Ioannis Tsivintzelis, and Georgios M. Kontogeorgis (Submitted for publication)
CERE 1503	"Hydrate Equilibrium Data for the CO <sub>2</sub> -N <sub>2</sub> System with the use of Tetra-n-butylammonium Bromide (TBAB), Cyclopentane (CP) and their Mixture" Fragkiskos Tzirakis, Paolo Stringari, Nicolas von Solms, Christophe Coquelet, and Georgios M. Kontogeorgis (Fluid Phase Equilibria, 408 (2016) 240-247)	CERE 1507	"Determination of Asphaltene Onset Conditions using the Cubic Plus Association Equation of State" Alay Arya, Nicolas von Solms, and Georgios M. Kontogeorgis (Fluid Phase Equilibria, 400 (2015) 8-19)	CERE 1511	"A Collocation Method for Surface Tension Calculation with the Density Gradient Theory" Peter Mahler Larsen, Bjørn Maribo-Mogensen, and Georgios M. Kontogeorgis (Submitted for publication)
CERE 1504	"Modeling Phase Equilibria for Acid Gas Mixtures using the CPA Equation of State. Part V. Multicomponent Mixtures Containing CO <sub>2</sub> and Alcohols" Ioannis Tsivintzelis, and Georgios M. Kontogeorgis (J. of Supercritical Fluids, 104 (2015) 29-30)	CERE 1508	"Permeability in Rotliegend Gas Sandstones to Gas and Brine as Predicted from NMR, Mercury Injection and Image Analysis" Esther Rosenbrand, Ida Lykke Fabricius, Quentin Fisher, and Carlos Grattoni (Accepted for publication)	CERE 1512	"Thermodynamic Modeling of Hydrogen Sulfide Absorption by Aqueous N-Methyldiethanolamine using the Extended UNIQUAC Model" Negar Sadegh, Erling H. Stenby, and Kaj Thomsen (Fluid Phase Equilibria, 392 (2015) 24-32)

CERE 1513	"Characterization Scheme for Property Prediction of Fluids Originating from Biomass" Thanh-Binh Nguyen, Jean-Charles de Hemptinne, Benoit Creton, and Georgios M. Kontogeorgis (Energy Fuels, 29 (2015) 7230-7241)
CERE 1514	"Measurement of Vapor-Liquid-Liquid Phase Equilibrium – Equipment and Results" Michael Frost, Nicolas von Solms, Dominique Richon, and Georgios M. Kontogeorgis (Fluid Phase Equilibria, 405 (2015) 88-95)
CERE 1515	"Mathematical Model for Enhanced Oil Recovery by Wettability Alteration Accounting for Oil Ganglia" Artem Alexeev, Alexander Shapiro, and Kaj Thomsen (Submitted for publication)
CERE 1516	"Investigation of Spore Forming Bacteria Flooding for Enhanced Oil Recovery in North Sea Chalk Reservoir" Amalia Yunita Halim, Sidsel Marie Nielsen, Anna Eliasson Lantz, Vural Sander Suicmez, Niels Lindeloff, and Alexander Shapiro (Journal of Petroleum Science and Engineering, 133 (2015) 444-454)





Martin Gamél Bjørner, Gürkan Sin, and Georgios M. Kontogeorgis (Fluid Phase Equilibria, 414 (2016) 29-47)



CERE 1533	"Nonlinear Multigrid for Reservoir Simulation" Max la Cour Christensen, Klaus Langgren Eskildsen, Allan Peter Ensig-Karup, Mark Wakefield (SPE 178428)	CERE 1537	"Pressure Dependence of the Solubility of Light Fullerenes in 1-hexanol from 298.15 K to 363.15 K" Konstantin N. Semenov, Teresa Regueira, Josefa Fernández, Nikolay A. Charykov, and Igor V. Murin (Journal of Molecular Liquids, 209 (2015) 71-76)	CERE 1541	"Dynamic Operation and Simulation of Post-Combustion CO <sub>2</sub> Capture" Jozsef Gaspar, Arne Gladis, John Bagterp Jørgensen, Kaj Thomsen, Nicolas von Solms, and Philip Loldrup Fosbøl (Energy Procedia, 86 (2016) 205-214)
CERE 1534	"Qualification of Polymer Materials for High Pressure CO <sub>2</sub> Flexible Pipe Structures" C. Wang, A. Rubin, N. Von Solms (SPE-FOTC-24468-MS (2013))	CERE 1538	"Time-Explicit Methods for Joint Economical and Geological Risk Mitigation in Production Optimization" Lasse H. Christiansen, Andrea Capolei, and John Bagterp Jørgensen (Submitted for Publication)	CERE 1542	"Control of a Post-Combustion CO₂ Capture Plant during Process Start-up and Load Variations" Jozsef Gaspar, John Bagterp Jørgensen, and Philip Loldrup Fosbøl (IFAC-PapersOnLine 48-8 (2015) 580-585)
CERE 1535	"On the Viscosity of Two 1-butyl-1-methyl- pyrrolidinium Ionic Liquids: Effect of the Temperature and Pressure" Félix M. Gaciño, María J.P. Comuñas, Teresa Regueira, José J. Segovia, and Josefa Fernández (J. Chem. Thermodynamics, 87 (2015) 43-51)	CERE 1539	<ul> <li><i>"Methods and Modelling for Post-combustion</i> CO<sub>2</sub> Capture"</li> <li>Philip Fosbøl, Nicolas von Solms, Arne Gladis, Kaj Thomsen, and Georgios M. Kontogeorgis</li> <li>(Submitted for publication in "Materials and Process Systems for CO<sub>2</sub> Capture: Modelling, Design, Control and Integration" edited by Dr. Athanasios Papadopoulos and Professor Panos Seferlis)</li> </ul>	CERE 1543	<sup>"</sup> Multivariable Optimization of the Piperazine CO <sub>2</sub> Post-Combustion Capture Process" Jozsef Gaspar, Nicolas von Solms, Kaj Thomsen, and Philip Loldrup Fosbøl (Energy Procedia, 86 (2016) 229-238)
CERE 1536	"Densities of the Binary Systems n-hexane + n-decane and n-hexane + n-hexadecane Up to 60 MPa and 463 K" Teresa Regueira, Wei Yan, and Erling H. Stenby (Journal of Chemical & Engineering Data, 60 (2015) 3631-3645)	CERE 1540	"Monte Carlo Reservoir Analysis Combining Seismic Reflection Data and Informed Priors" Andrea Zunino, Klaus Mosegaard, Katrine Lange, Yulia Melnikova, and Thomas Mejer Hansen (Geophysics, 80(1) (2015) 31-41)	CERE 1544	"Pitfalls of using the Geometric-mean Combining Rule in the Density Gradient Theory" Xiaodong Liang, Michael Locht Michelsen, and Georgios M. Kontogeorgis (Submitted for publication)

CERE 1545	"Modelling the Phase Equilibria of Multicomponent Mixtures Containing CO <sub>2</sub> , Alkanes, Water and/or Alcohols using the Quadrupolar CPA Equation of State" Martin G. Bjørner, and Georgios M. Kontogeorgis (Submitted for publication)
CERE 1546	"A Dynamic Mathematical Model for Packed Columns in Carbon Capture Plants" Jozsef Gaspar, John Bagterp Jørgensen, and Philip Loldrup Fosbøl (Proceedings from 2015 European Control Conference, (ECC), July 15-17, 2015, Linz, Austria)
CERE 1547	"Profit and Risk Measures in Oil Production Optimization" A. Capolei, B. Foss, and J.B. Jørgensen (IFAC-PapersOnLine, 48-6 (2015) 214-220)





As a university research center, our goal is to spend all of our money on research. No management bonuses or other dividends are due, and 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 postdoc level.

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