

# CERE

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## CERE Annual Report 2014

### **Publisher:**

CERE, Center for Energy Resources Engineering  
Technical University of Denmark (DTU) Building 229  
DK-2800 Kgs. Lyngby, Denmark

**Phone:** +45 45 25 20 12

**Fax:** +45 45 88 22 58

### **Website:**

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

### **Editor-in-chief:**

Georgios Kontogeorgis, Chairman of CERE

### **Assistant Editors:**

Patricia Wagner, Project Administrator, CERE

Anne Louise Biede, Secretary, CERE

### **Text:**

Morten Andersen, science reporter

[www.manjournal.dk](http://www.manjournal.dk)

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### **Photos - unless otherwise stated:**

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06

**Evaluation, Expansion and Excitement**

In his first address as Chairman of CERE, Georgios Kontogeorgis introduces this years' report.

08

**Challenges of high Complexity**

Shale gas, CO<sub>2</sub> based Enhanced Oil Recovery, and oil and gas exploration at large depths, are examples of the topics at the CERE Discussion Meeting 2014.

10

**The Stenby Equation of State**

Stepping down after 20 years as head of CERE, Professor Erling H. Stenby reflects on successes and bumps on the road.

12

**Strength from Industry Participation**

Input from close to 30 international industry partners ensure that CERE activities are relevant to the topical problems and limitations in existing knowledge.

14

**Important finding in Microbial Enhanced Oil Recovery**

According to CERE laboratory tests, bacteria can increase recovery by 4-7 % over water flooding in tight carbonate reservoirs.

16

**Proteins from Nature as Hydrate Inhibitors**

Anti-freeze proteins found in insects, worms and Arctic fish species can inhibit the formation of gas-hydrates, which are a nuisance to oil and gas recovery.

18

**A Hydrate Energy Future?**

According to the US Geological Survey, the amount of methane captured inside hydrates exceeds the world's presently known gas reserves.

20

**Powerful Software for Advanced Thermodynamics**

CERE has turned its academic findings into a software portfolio useful to fields such as oil exploration and recovery, complex mixtures including electrolytes, and carbon capture.

22

**News from CERE**

A new consortium with CERE in a leading role is to create a platform for converting biomass into high-value energy resources. Also, the purchase of advanced equipment for HPHT (High Pressure, High Temperature) research is reported in the brief news section.

26

**PhD Theses of the Year**

2014 was a highly fruitful year in regards to PhD degrees – no less than 8 theses were successfully defended.



# A Year of Evaluation, Expansion and Excitement



Welcome to the 2014 CERE Annual Report. It has been a truly exciting year in several ways. 2014 was the 5th year of CERE as an interdisciplinary engineering center in energy resources with special emphasis on petroleum applications. To mark this - and also to plan the future - an international research evaluation was conducted. I want to express our sincere thanks to the committee - Professor Arne Skauge, CIPR, Norway (chairman of the committee); Professor Tor Arne Johansen, University of Bergen, Norway; Dr. Oliver Koch, Linde Engineering, Germany; and Dr. Jose A. Torres, ConocoPhillips, USA - for their excellent work resulting in a comprehensive report. The findings will be discussed internally, and indeed one of the numerous good suggestions has already been implemented - namely a Newsletter to the Consortium; launched by late October 2014.

2014 also marked a change in the leadership of the center. Starting July 1, I have accepted the position as Chairman of CERE, succeeding Professor Erling H. Stenby who was the head of the center for about 20 years. There is little doubt that the center's (both in the forms of IVC-SEP and of CERE) success and appeal to industry is owed to a very large extent to Erling's efforts, dedication and excellent leadership over this very long period. Some of Erling's reflections on these 20 years can be read in this report. It is, thus, both an honour and a great responsibility to take over this position. I am confident that we will succeed, with the contributions of a team of dedicated faculty and researchers, assisted by our skilled technical and administrative personnel.

Erling will contribute to the center in the years to come via the many CERE projects he is involved in or coordinating. He will also be busy with other duties, as of July 1 he has undertaken the role of Scientific Director in the newly formed Danish Hydrocarbon Research

and Technology Center. The establishment of a center funded by the Danish Underground Consortium, with focus on Danish oil & gas resources was an important development during 2014. At CERE we will continue our research activities in the broader petroleum engineering field and associated disciplines at the international arena, whereas we both hope and expect synergy and a fruitful collaboration with the new center on projects of mutual interest.

At CERE we have projects covering a wide portfolio often combining the diverse disciplines of the center - chemical engineering, applied chemistry, scientific computing, geology, and geophysics. This report presents some of the most successful projects during the year covering several of the areas we are working in. I hope you will appreciate the developments we present in enhanced oil recovery, hydrate inhibitors and some of our most successful software.

We have often stated that our PhD students and post-doctoral researchers are possibly the most important "product" of the center. We are proud to be able to attract talented people from all over the world in this highly competitive international environment. 2014 has been a special year in this direction as 8 of our PhD students have successfully defended their theses. We follow their subsequent careers with interest and we are happy when several of them continue collaborating with the center, either from academic positions or from the companies they are employed by. It was nice to see several of "our" people returning as member company representatives at the CERE Discussion Meeting.

Further, let me mention that CERE will continue expanding, trying to attract the interest of new member companies, funding for new projects - also within areas we may not have engaged in before - and last but not least attracting new co-workers, including faculty and researchers.

We already know that in 2015 we will welcome two new companies, Calsep and Union Engineering, to the CERE industry consortium. Further, we will co-ordinate a new project (recently granted by Innovation Fund Denmark) on converting biomass into high-value energy resources. In this project our skills on engineering design will be combined with the skills of the project partners in other areas such as gasification, fermentation, separation, etc. This will be yet another interdisciplinary project in CERE.

Finally, CERE will welcome new faculty members in 2015. One of them is already known. It is Associate Professor Allan Peter Engsig-Karup from DTU Compute. Allan is already involved in the OPTION project of CERE (see the 2013 report) and we believe he can contribute significantly in CERE's future development. We are excited that he has accepted to join CERE.

I hope you will enjoy the report. Should you have comments or questions I will appreciate if you contact me. Feedback and discussion are very important for our future development.

Much has happened in 2014! It has indeed been an exciting year!

We look forward to an equally exciting 2015 and I hope to see you at the annual CERE Discussion Meeting at Comwell Borupgaard, Snekkersten 17-19 June 2015.

Professor Georgios Kontogeorgis,  
Chairman of CERE



# CERE Discussion Meeting 2014

## Energy Challenges of high Complexity

Shale gas, CO<sub>2</sub> based Enhanced Oil Recovery, and oil and gas exploration at large depths, are examples of the challenging issues represented at the CERE Discussion Meeting 2014.

With no less than 40 external participants, representing 19 energy corporations and other industry from 13 countries, the 2014 version of CERE's Discussion Meeting was yet another summit of energy resources engineering.

Several sessions were devoted to unconventional carbon-hydrate resources, and to conventional recovery under high pressure or otherwise challenging conditions.

"Such complex issues have always appealed to academia, but actually I find this focus is also reflecting the demands of industry. Shale gas, HPHT, and otherwise challenging resources are becoming an ever larger part of the business," according to Dr. Vural Sander Suicmez, senior reservoir engineer at DBU Subsurface Development, Maersk Oil.

Dr. Suicmez attended the Discussion Meeting for his first time.

"I am pleased that the Discussion Meeting is open to industry suggestions. The broad range of participating companies implies that no single company can expect to have all its wishes fulfilled. This is a fact that I am happy to accept, since it is really beneficial to have a wide range of companies in the Consortium."

## Reality check in flow assurance

Headquartered in Houston, Texas, Chevron Energy Technology develops and manages technology to help find and produce new oil and gas reserves, enhance recovery in existing fields, and optimize productivity of downstream assets.

"One of the advantages of being in the CERE industrial Consortium is that we get access to new simulation tools. Modern recovery takes

place under complex conditions, often under very high pressures, and it is just not possible for us to measure everything," explains Dr. Samer O. Derawi, senior flow assurance engineer at Chevron.

"Besides modelling, which is one of my job responsibilities within Chevron, we are also keen to take advantage of independent experimental results. We rely on conventional anti-freeze chemicals for flow assurance, primarily for inhibition of gas hydrate formation. Often we will be approached by the chemical vendor who claims to have developed improved versions of their products. Is this true or not? CERE can provide us with a reality check."

Dr. Derawi follows the efforts at CERE around inorganic scale and low dosage hydrate inhibitors with special interest. "Presently we trust the conventional products, but it would be interesting for us if alternative inhibitors can be found which will be effective in much smaller volumes."

## A fine venue for recruitment

With a staff above 120,000 worldwide, Oil Field Services consultants Schlumberger is a major employer in energy engineering, not least in the fields addressed by CERE.

"The Discussion Meeting is a fine opportunity to meet young people that could be interesting for us to recruit," says Dr. Simon Ivar Andersen of Schlumberger, adding smilingly:

"And also people that are not quite so young."

"Further, CERE has always been dynamic and able to generate collaboration and attract funding. For instance the new center for applied oil and gas research at DTU (the Danish Hydro-carbon Research & Technology Centre, Ed.) has strong participation from CERE. It is something that is followed with great interest from people in the business, also outside Denmark."



## Norway leads in carbon capture

Gassnova, the Norwegian state enterprise for CCS, advises the Norwegian Ministry of Petroleum and Energy on CCS and manages the state interests in related projects. The company is the majority owner of Technology Centre Mongstad (TCM), which has been in operation for about two years and has operated the project planning of full scale projects like Kårstø and Mongstad. TCM has two carbon capture testing facilities, which combined has a capacity of 100,000 tons of CO<sub>2</sub> yearly. These activities are at the forefront of international CCS development.

"The group at CERE is known for developing thermodynamic models that are very useful for us. Experimental testing is costly. Each time you can achieve your results by computing instead you have saved a lot of money," says Dr. Muhammad Ismail Shah of Gassnova.

"Especially the developments in models that are able to handle CO<sub>2</sub> capture, including the chilled ammonia process which is used at one of the two Norwegian plants, and electrolyte systems are of great interest to us. CERE is providing us with good tools, and we provide them with actual plant data – non-confidential - which they can use for validating their models. Both sides are necessary for obtaining the overall understanding of the processes and for developing still better tools for simulation and design of carbon capture facilities."

## The French connection

With more than 1,600 employees and a plus 300 million EUR budget, the IFP Energies Nouvelles is one of the leading players in energy innovation in France.

"In many respects what we do in my department is similar to what is done at CERE, for instance within thermodynamics, EOR, geology, geophysics, and other fields. Thus

it is highly beneficial to cooperate," says Dr. Pascal Mougou of IFP Energies Nouvelles.

"To give an example, I have just learned that CERE is initiating a project very similar to one we are about to start. Both parties can gain from coordinating the academic background core for the experiments. Another joint activity is the exchange of students. We have had a few exchanges and are looking forward to more."

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*The CERE Discussion Meeting 2014 was held from June 25 – June 27 2014 at Comwell Borupgaard, Snekkersten. 40 external participants representing 19 companies, 3 foreign university groups, and 13 nationalities attended.*

CERE Discussion Meeting 2015



Read more about the CERE Discussion Meeting 2015





Stepping down after 20 years as head of CERE, Professor Erling H. Stenby reflects on successes and bumps on the road.

By July 2014 Erling H. Stenby changed his status from head of CERE to one of its closest partners. Holding a dual position as Head of Department at DTU Chemistry and Scientific Director at the newly created Danish Hydrocarbon Research and Technology Centre, he hands over the leadership of CERE while maintaining his professional interest and participation in the research of the center.

During his 20 years of leadership, CERE has grown from a small research group within applied thermodynamics to a broad center involving faculty from five DTU departments and attracting 5.5 million EUR annually in external funding.

“We have grown but at the same time always resisted the temptation to engage opportunistically in fields that have been “hot” at a given moment. This could have yielded

further short-term growth, but would also have made us vulnerable to fluctuations in political interest. Instead we have maintained a broad portfolio based on our fundamental competencies within applied thermodynamics and bordering fields. This allows me to say with confidence that the center is in a robust condition.”

#### Research policy shock in 2001

The value of a diversified strategy truly became visible in 2001, when a change of government was followed by dramatic cuts in Danish public funding for research related to energy and environment. One of the consequences was the termination of publicly funded hydrocarbon research under the Danish Energy Agency. “This was a shock to us, as it was to several other groups. But fortunately, we were able to maintain our commitment in this field.”

Since 1988 the group had been organized as a center of fundamental research, the Center for Phase Equilibria and Separation Processes, funded by the Danish Research Councils.

## The Stenby Equation of State

“The basic funding for this center was very important. Also, we were able to “gear” the funding with contributions from the members of our industry Consortium.”

A further source was the EU which only later abandoned hydrocarbon research.

“So in essence we were able to keep up our efforts within oil and gas research, despite the field being in bad standing several places in the public research funding system.”

#### Building trust with industry

The previously hostile official attitude towards hydrocarbon research is currently under revision as indicated by the new Danish Hydrocarbon Research and Technology Centre. The center is headquartered at DTU, and will involve academic resources at three other Danish universities plus the national geological survey, GEUS. The partners of the Danish Underground Consortium (DUC) have provided the centers’ funding of DKK 1.0 billion over 10 years.

“...we have maintained a broad portfolio based on our fundamental competencies within applied thermodynamics and bordering fields. This allows me to say with confidence that the center is in a robust condition.”

Erling H. Stenby is Scientific Director for one of the three “legs” of the new national center, namely that of Enhanced Oil Recovery (EOR).

“Obviously, there will be a strong collaboration between the new national center and CERE for example around CERE’s Joint Industry Projects - SmartWater, BioRec, NextOil, and others.”

Looking back over the 20 years it is especially the involvement of the joint projects with industry which stands out.

“Joint projects with industry are main stream at the Danish universities today, but 20 years ago that was far from the case. Also, we need to remember that the relations with industry are assets. It takes time to develop this kind of mutual trust and respect.”

In other words, other groups and institutions can’t expect to replicate these relations easily.

“No, and I would also like to add that this also goes for industry. If a company just sees the university as a cheap know-how service provider things are bound to go wrong.”

#### Carbon capture and thermal energy

The 2001 cut-down on Danish public energy research encouraged the CERE management to strive for further diversification.

“We knew that our competencies within thermodynamics were highly relevant to Carbon Capture. We could therefore contribute to combating climate change caused by carbon dioxide emissions from coal fired power plants and other sources. And when members of our industry Consortium confirmed an interest in the field, we moved ahead,” Erling H. Stenby recalls.

After the failure in 2009 to establish an international consensus on climate change, political interest in Carbon Capture has declined somewhat. However, CERE maintains

a certain amount of activity, mostly based on EU funding.

“Internationally, carbon capture is put on hold, but the minute things start moving ahead again, CERE is ready.”

Similarly, geo-thermal energy is going through a dry spell, at least in Denmark.

“The absence of a national strategy for geo-thermal energy makes it difficult for the energy sector to move ahead full-speed, but once it happens, CERE can contribute. And the same can be said for shale gas. Both fields are projected to have a large potential in Denmark, but await political clarifications.”

“So, in all these fields I have not regretted our commitment.”

#### A few regrets

But surely, in 20 years there must be some regrets? Erling H. Stenby has to think for a minute, then replies:

“A few years ago we started activities on large-scale flowing batteries. These are relevant in various sustainable energy contexts like storage of excess power from wind turbines. We abandoned the activity due to lack of external funding. However, I feel we might have tried harder on this.”

“A similar case was bio-thermodynamics. We did have a project on optimization of pharmaceutical production, and currently Novo Nordisk is implementing methods similar to those investigated in the project. Again, I feel we could have tried harder to maintain this activity in CERE.”

The project on bio-thermodynamics would also, had it been continued, have strengthened the non-energy related activities in CERE.

“At the outset the Center for Phase Equilibria and Separation Processes was actually more

focused on chemical industry than on energy. Things could have gone either way.”

#### Broad scope secures robustness

In 2009, the dominant status of the energy related activities was reflected as the name was changed from the previous name to Center for Energy Resources Engineering – CERE.

“Still, it is important that the center has a broad scope within energy applications. I have also taken pride in the fact that we have engaged in projects that are not main stream energy resources projects. A project on utilization of fly ash from biomass energy production as fertilizer was an example.”

The change in 2009 was truly a highlight to Erling H. Stenby:

“It was a truly remarkable day as the scope was broadened to include faculty from departments outside DTU Chemical Engineering. We soon saw how it became possible to start Joint Industry Projects such as SmartWater, BioRec, and NextOil – all highly interdisciplinary. All in all, I think it is fair to say, that the expansion has built yet another layer on top of the core competencies in CERE. This should contribute further to the robustness of the center.”

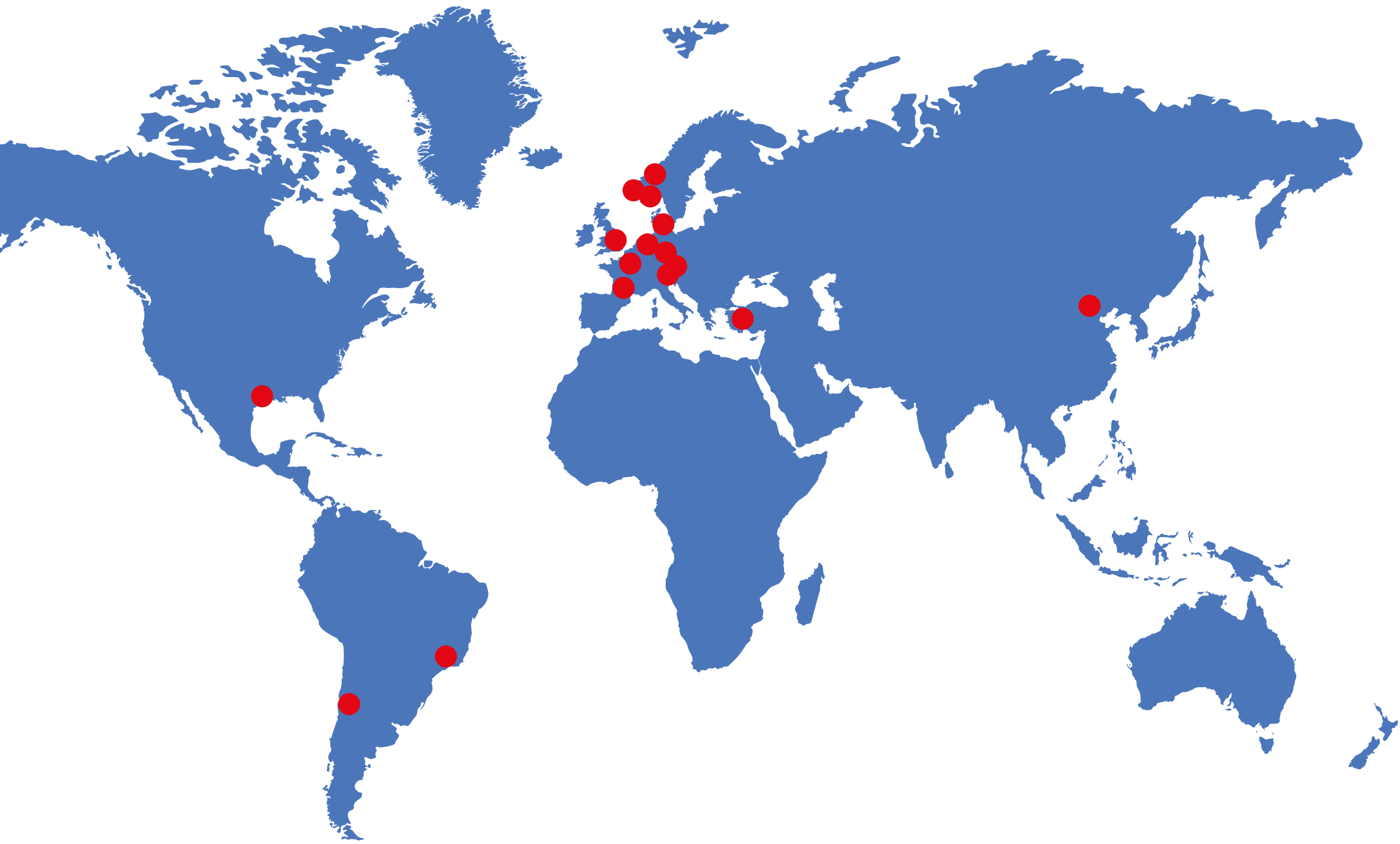
# The Consortium - our Strongest Asset

CERE is supported by public means from several sources, e.g. The Danish Council for Independent Research - Technology and Production Sciences, EU's FP7, and The Danish National Advanced Technology Foundation. Furthermore the center is supported by grants from several private companies. The strongest asset of CERE is

the industrial Consortium. Approximately 25-30 companies are members, the exact number changes due to the dynamics of the industry's mergers and acquisitions.

The member companies closely follow the activities of 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 Genel Energy**

Genel Energy is an Anglo-Turkish oil and gas exploration and production company. The company's core assets are located in the Kurdistan region of Iraq, where the Taq Taq and Tawke fields have estimated reserves of 1.3 billion barrels of oil, and 1.8 billion barrel equivalents of gas. Further, Genel Energy is building a broader exploration portfolio through value-accretive acquisitions in other Middle East countries and in Africa.

AkzoNobel Research, The Netherlands  
BP Chemicals Limited, United Kingdom  
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  
Genel Energy, Turkey  
Haldor Topsøe A/S, Denmark  
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  
National Oilwell Varco Denmark I/S, Denmark  
OMV E&P, Austria  
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SINOPEC, P.R. China  
SQM SA., Chile  
Statoil, Norway  
TOTAL, France  
Welltec, Denmark



# Chinese Bacteria can help North Sea Oil Recovery



Amalia Yunita Halim  
PhD Student

Injection of the bacteria *Bacillus licheniformis* is able to increase recovery rates by 4 % in core samples from the Danish North Sea compared with the traditional oil recovery method, which is water flooding. And smart application of bacterial injection to complex petroleum reservoirs may yield an even better result - a 7 % increase.

The experiments are done in the framework of the BioRec project (Biotechnology in Oil Recovery) at CERE as a part of Amalia Yunita Halim's PhD. project on microbial enhanced oil recovery (MEOR).

In any type of business a 4-7 % increase in production would be of interest. And when

it's oil exploration, we are talking about billions of dollars worth. No wonder Amalia Yunita Halim has felt interest from energy corporations Maersk Oil and DONG Energy, both BioRec industry partners:

"Both companies have followed the project closely. We have held meetings with our partners three times a year, and we have also received feedback in-between meetings. They have provided us with the actual core samples from the North Sea but also with input and suggestions that have been useful in planning our experiments."

## Industry has inspired a dual strategy

An example of how industry input has proved valuable is the question of how MEOR should be combined with water flooding. "Petroleum reservoirs are often developed by water flooding until production of oil becomes insufficient or negligible. This is a moment where companies usually think about application of the different EOR methods, including microbial enhanced oil recovery. However, MEOR may start earlier, when the reservoir potential has not yet been exhausted. This may result in additional recovery," says Amalia Yunita Halim, adding that bacteria may be especially helpful for the reservoirs with variable properties – which the majority of reservoirs have. A combined method yields the best results – 7 % increase – while application of MEOR after reservoir exhaustion "only" increases recovery with 4 %, so it seems natural to dedicate further research to the combined method.

"However, for various practical reasons it could be easier in some cases to apply MEOR alone to fields that have been shot down, rather than combining bacteria and water flooding in operational fields. Therefore we have decided to continue with a focus on both scenarios, as they are both highly relevant to the industry," Amalia Yunita Halim explains.

## Biotechnology in Oil Recovery

The BioRec program (Biotechnology in Oil Recovery) was initiated in 2012. The program is coordinated by CERE. Industry partners are Maersk Oil, DONG Energy, and Novozymes. Academic partner is Danish Technological Institute (DTI). The program has an overall budget of EUR 4.5 million, where EUR 2.0 million was provided by the Danish Advanced Technology Foundation (today the Danish Innovation Foundation), EUR 1.5 million by the industry partners, and EUR 1.0 million by DTU. The program consists of three work packages. The package on microbial and enzymatic oil recovery is coordinated by Associate Professor Alexander Shapiro, DTU Chemical Engineering, while the package on inhibition of gas hydrate formation is coordinated by Associate Professor Nicolas von Solms, DTU Chemical Engineering, and the package on prevention of microbial induced corrosion by DTI. Overall BioRec coordinator is Professor Erling H. Stenby, DTU Chemistry.

## Known from Chinese reservoirs

aim of all types of Enhanced Oil Recovery (EOR) is to extend the productive life of otherwise depleted and uneconomic oil fields. EOR is usually applied after more conventional methods, primarily pressure depletion and water flooding, have been exhausted. While most commonly either chemicals, gas or steam are injected into the reservoir, over the latest years biological EOR techniques have gained increased attention all around the world.

Manipulating microbial communities is actually not unknown to the oil industry. The idea of adding nutrients which stimulate growth of certain indigenous microbes in order to increase production has been documented as early as the 1950'ies. For example in some fields, where growth of sulphate-reducing microbes would cause souring problems, it is an established method to inject nitrate blended with the injection water. This stimulates growth of nitrate-reducing microbes which limits the growth of sulphate-reducing microbes.

However, the approach investigated by Amalia Yunita Halim is more radical, as it introduces exogenous microbes to Danish North Sea rock types. From the outset also indigenous and also other exogenous species were looked at, but for some time the prime focus has been the *Bacillus licheniformis*. The actual form of the organism, type 421, has been isolated from reservoirs in China.

## Can survive despite scarce nutrition

A number of experiments have showed the potential of the bacteria for MEOR in the North Sea.

Firstly, it was important that the bacteria could penetrate into the tight carbonate formations known from several Danish reservoirs. This was by no means a given thing as the size of the bacteria is almost comparable to the pore throat size of the chalk. Fortunately the experiments showed that it is indeed possible to introduce the bacteria. The

microbes are flexible to a point where they can even adjust the shape of the individual cells, allowing them to penetrate at critical pore sizes.

Secondly, the *Bacillus licheniformis* is spore-forming, which is practical since this ability largely increases its chances of survival. Should the organism be caught in a location with scarcity of nutrition, it will form spores that are able to sit or travel idle until conditions later improve.

Thirdly, and indeed importantly, experiments were done to prove that the bacteria were actually able to increase recovery rates. This is now documented. In oil saturated rock samples from the Danish North Sea it proved possible in the lab to extract 54 % average by water flooding, while the similar figure was 58 % by *Bacillus licheniformis* MEOR, and 61 % by applying a combination of water flooding and MEOR.

## Plugging is a possible mechanism

Not only are the results highly interesting to industry, they also spur further academic work.

"Obviously, we would like to be able to explain the mechanism behind the increased output," Amalia Yunita Halim notes.

In cooperation with CERE co-workers, postdoc Sidsel Marie Nielsen and Associate Professor Alexander Shapiro, she currently investigates a suggested mechanism.

After primary oil recovery, the larger channels of the rock have typically been emptied, and the remaining oil sits in tight, smaller channels. When water flooding commences it will produce some extra oil, but not that much because the water will tend to flow through the larger, empty channels. As the bacteria are introduced they will inhabit the larger channels, forcing the water to penetrate the smaller, oil-rich channels and drive the oil out. The phenomenon is known as selective plugging.

"We hope to be able to confirm this mechanism in future work, by combining the experimental results with modelling that Sidsel Marie Nielsen does. It is one of the strengths at CERE that we are able to combine different disciplines in this manner," says Amalia Yunita Halim.

## Will face competition from local bacteria

A further topic, which is important but has not yet been investigated, is how well the bacteria will survive the competition which it will inevitably meet from the indigenous microbes. The indigenous microbes are studied in collaboration with the Danish Technological Institute (DTI), also a partner to the BioRec program.

The cooperation with DTI has identified three types of indigenous microbes which are dominant in the Danish North Sea reservoirs, and which the *Bacillus licheniformis* will primarily have to compete against for nutrients. The next step will be to set up experiments that clarify how well the *Bacillus licheniformis* is suited for this competition. Should it prove to suffer, it could then be considered if certain nutrients should be introduced jointly with the microbe to increase the chances for survival of the new MEOR candidate.





# Proteins from Nature are able to Inhibit Hydrate Formation

Anti-freeze proteins found in insects, worms and Arctic fish species can inhibit the formation of gas-hydrates, which are a nuisance to oil and gas recovery. The efficacy is on a level with commercially available synthetic inhibitors, and the environmental advantages are large.

A headline in the 2009 CERE Annual Report read “Proteins from Nature May Replace Synthetic Gas Hydrate Inhibitors”. Today, the word “may” can safely be deleted and replaced with “are able to”. The 2009 article announced the start of a project in the field at CERE. In 2014, the project demonstrated that the idea works. This means that naturally occurring proteins can become serious candidates for gas-hydrate inhibition in oil and gas recovery – especially in areas where the use of highly effective, synthetic inhibitors is forbidden or restricted due to bio-degradability concerns. This is for instance the case in the North Sea.

“We still have issues to work on. First of all the proteins are currently too expensive. This is not surprising, as so far they have been manufactured only in tiny volumes for laboratory experiment purposes. When the production is scaled up the price will obviously come down. However, it is beyond the scope of CERE’s research to optimize protein production,” says Associate

Professor Nicolas von Solms, who has headed the research at CERE.

Taking the proteins closer to large-scale production is currently a task for the Department of Science, Systems and Models at Roskilde University, a partner in the project.

## Hydrates cause huge losses

The summit of the research project was the publication in May 2014 by the scientific journal “Energy Fuels” (American Chemical Society) of a study on a protein from the Longhorn Beetle (*Rhagium mordax*).

The article, with PhD student Christine Malmos, CERE, as lead author, showed that the protein RmAFP1 (*Rhagium mordax* anti-freeze protein 1) is able to inhibit hydrate formation as effectively as polyvinylpyrrolidone (PVP). PVP is an efficient, commercially available synthetic polymeric inhibitor.

“The work has been laborious since gas hydrate formation is not a linear process. There is a large stochastic component, which means that we have had to perform a large quantity of experiments to obtain statistically satisfactory results. But the article demonstrates the efficacy of RmAFP1 beyond any doubt,” says Nicolas von Solms, senior author on the article.

Gas hydrates are substances resembling snow or ice consisting of water and light hydrocarbons. Under certain conditions they will precipitate in pipes and production gear. This again may lead to production stops implying major economic losses. A combination of low temperature, high pressure and presence of water is known to provide ideal conditions for hydrate formation. Unfortunately those are exactly the conditions under recovery at Northern locations or deep water. Presently large quantities of inhibitors, primarily methanol and ethylene glycol, are utilized.

## Acts as a “negative catalyst”

Methanol and glycol are so-called thermodynamic inhibitors (THIs), meaning they work by lowering the temperature point at which hydrate formation starts. This is similar to the way the same substances are used in vehicles to lower the freezing point of water. By adding THI’s the hydrate phase boundary is shifted towards lower temperatures, meaning lower temperatures will be required to form hydrates for a given operating pressure. THI’s must be added in high dosage concentrations. 20-50 wt % concentration of methanol or glycol is commonly seen in the fluid phase under recovery and transportation of oil and gas at Northern locations. Such large quantities add to costs and also pose several

environmental and safety challenges related to storage, transportation, and handling. An alternative class of chemicals, kinetic hydrate inhibitors (KHIs) has been developed. Rather than lowering the temperature point of hydrate formation, a KHI acts as a negative catalyst which inhibits key chemical processes involved. Currently, water-soluble polymeric compounds are used as KHIs, and their prime advantage is that they can be applied in much lower concentrations (0.1-1.0 wt %) than THIs. PVP is one of them.

Despite the efficacy of KHIs they have not been accepted everywhere, mainly due to bio-degradability concerns. For instance, they have not been certified for use in the North Sea. This is the primary motivation for the research project on possible alternatives.

## Essential input from industry partners

A number of animal species have anti-freeze proteins. While the freezing of water and hydrate formation are not exactly the same processes there are a number of chemical similarities, so one would assume that the same substances that help fish survive in cold water, or insects to survive during winter may also inhibit hydrate formation. In fact, the commercially available polymers were inspired by deep sea fish proteins from the outset.

The project at CERE was soon extended and integrated into the joint industry project BioRec, which investigates several aspects of putting biology to use in oil and gas recovery. Industry partners are DONG Energy, Maersk Oil, and Novozymes.

“The significant economic contributions from industry have been essential for the project. Further, the two energy partners have provided us with actual data from production. These have been highly valuable in assuring that our laboratory experiments are relevant to real conditions,” says Nicolas von Solms.

## A robust and efficient protein

The Department of Science, Systems and Models at Roskilde University is the academic partner to CERE in the project. The department pioneered anti-freeze studies on the *Rhagium mordax* beetle, and has set up an RmAFP1 production by *E. coli* fermentation.

“Their contribution has been essential, as they were able to provide the RmAFP1 in the quantities needed. The experiments showed that the protein is remarkably efficient as a hydrate inhibitor. The group at Roskilde University has also shown that the protein can tolerate heating. This is a key technical parameter once the protein will be subject to use in actual recovery,” says Nicolas von Solms.

The experiments have shown that addition of RmAFP1 in a low concentration (2,770 ppm) decreased the nucleation temperature (the temperature where hydrates begin to form) from 11.5 to 8.6 °C under realistic high-pressure conditions. This was comparable, and in fact slightly better, held against the benchmark commercially available inhibitor PVP which was able to lower the nucleation temperature to 9.0 °C.

The project on anti-freeze proteins as hydrate inhibitors was supported by The Danish Council for Independent Research – Technology and Production Sciences, the Danish National Advanced Technology Foundation, and DTU.





## A Hydrate Energy Future?



Nicolas von Solms  
Associate Professor

According to the US Geological Survey, the amount of methane captured inside hydrates exceeds the world's presently known gas reserves.

"Methane extracted from hydrates could become a major energy source in the future. Based on our experience with gas hydrate research we are in a good position to take part in this quest," says Associate Professor Nicolas von Solms, CERE.

Just by the beginning of 2014, the Geological Survey of Denmark and Greenland (GEUS), announced gas hydrate findings in the Disco Bay in Western Greenland.

"We noticed the finding with great interest. It is natural to look for hydrates in cold regions like Greenland, but actually one can expect to find them all over the globe, especially along the ocean margin zones where conditions are generally favorable for hydrate formation," Nicolas von Solms comments.

Sceptics have argued that production costs will be too high, as it will be difficult to produce methane in deep waters without having it leaking to the surroundings. Also, one needs to be concerned about the consequences for rock stability once production begins, Nicolas von Solms underlines:

"There are a number of issues that need to be addressed, and it is too early to say whether production will become realistic. Still, many of the same negative projections were made regarding shale gas just a decade ago, and today this has become a major energy source. The same thing might just happen for gas hydrates."

## Carbon Capture by Gas Hydrates

While energy corporations are hardly enthusiastic about having gas hydrates in their production gear for oil and gas recovery, the matter is totally different when it comes to finding the same substances in carbon capture units at coal fired power plants.

"Combining flue gases from coal fired power plants with gas hydrates would be a win-win situation," explains Associate Professor Nicolas von Solms, CERE.

A gas hydrate molecule is in effect a "cage" in which a small molecule, most commonly methane, is trapped. Carbon dioxide is capable of acting as an agent which drives methane out from its shelter. If the process is designed smartly, the carbon dioxide molecule will be caged instead. The result would be a dual benefit. The valuable methane will be gained, while the carbon dioxide, which is unwanted in the atmosphere, would be captured.

Further, experiments have shown that this "hydrate swapping" may readily take place, and also that gas hydrates have an extra benefit. It is a major challenge in carbon capture that flue gas, just as atmospheric air, consists mainly of nitrogen. The handling of the large quantity of nitrogen normally leads to a large energy

consumption which damages both the economy and the climate friendliness of the operation. However, the gas hydrates are highly selective for carbon dioxide, meaning they will allow nitrogen to pass unhindered and thus effectively function as a filter for carbon dioxide.

"At least theoretically, gas hydrates are ideal for carbon capture. However, large practical challenges need to be overcome," says Nicolas von Solms.

The top challenge is the fact that gas hydrates are formed under low temperature and high pressure, while the flue gas at a power plant presents just the opposite conditions.

"You may say that we have the kinetics working against us here. With presently known technology a reactor for capturing carbon dioxide by use of hydrates would have to be so large, that the whole project would just become way too costly." Thus, the scientific efforts are focused on techniques that promote hydrate formation. In other words the aim is to allow hydrate formation to take place at higher temperature and/or lower pressure than usual. In his PhD. project at CERE, Peter Jørgensen Herslund has demonstrated that a mixture of cyclopentane and tetrahydrofuran (THF) was able to act as a promotor. By adding 5 mol% of THF to the aqueous phase of a cyclopentane system,

hydrate dissociation pressures were reduced by approximately 20 % compared to those measured for the cyclopentane promoted system at similar temperatures. In other words, the two compounds showed a synergistic effect.

"We were pleased to see this synergistic effect, especially since we had predicted the effect from thermodynamic modelling. It is one of the rare occasions where a theory is later confirmed by experiments rather than developing a theory to fit observed data," says Nicolas von Solms, who co-supervised the project with Associate Professor Kaj Thomsen.

An article establishing the synergistic effect of cyclopentane and THF as a thermodynamic carbon dioxide hydrate promoter was published in the journal "Fluid Phase Equilibria" (Elsevier) August 2014.

*The work on carbon capture by gas hydrates was supported by the European iCap project under the 7th EU frame work program for science and innovation, and DTU.*



# Powerful Software for Advanced Thermodynamics



Alay Arya  
PhD Student and  
Software Manager

CERE has turned its academic findings into a software portfolio useful to fields such as oil exploration and recovery, complex mixtures including electrolytes, and carbon capture.

Some years ago, CERE took a strategic decision. The researchers were already using various home-brewed types of software especially within thermodynamic modelling. It seemed evident that these in-house tools could be turned into products with broader application if the necessary resources were put into improved user-friendliness and verifications.

“The products are in high demand, especially from the members of our industry Consortium,” says Alay Arya, holding a dual position as PhD. student and software manager at CERE. Further, he is responsible for the continuous development of one of the software products, the ThermoSystem.

“The product enables the use of our thermodynamic models as add-ins to process simulators, such as Aspen HYSYS, used by industrial partners,” Alay Arya explains. “As the models are not yet implemented in commercial process simulators, ThermoSystem reduces the gap between on the one side the industrial engineers that use thermodynamic models

for process simulation, process optimization, and process control and on the other side the scientists at CERE that develop the models.”

## Updates without user efforts

The ThermoSystem builds on an advanced thermodynamic model, the Cubic Plus Association (CPA) equation of state, which has been developed by CERE in cooperation with the partners in the Joint Industry Project CHIGP (Chemicals in Gas Processing). The CPA extends the classical cubic equations of state used in the oil and gas industry to account for the various chemicals used in modern exploration and recovery for hydrate inhibition and other purposes.

A standard version of the ThermoSystem is available to all members of the CHIGP Consortium free of charge, while extended functionalities can be bought.

Unlike most commercial software providers, CERE does not issue frequent new versions of ThermoSystem to generate sales.

“We improve the software continuously by including new components and new parameters, as the science progresses, but we can do that just by updating our database, meaning that users do not need to install new versions of the software,” says Alay Arya.

## Know your scaling

Another popular CERE product is software for calculating solubility equilibrium under pressure. Formation water is usually saturated with minerals of the surrounding reservoir

rock. During oil production may temperature, pressure and composition of the brine change, causing precipitation of some of these salts. This is called scale formation or scale deposition. When formation water is mixed with other brines, some salts may become supersaturated and form scale too.



Kaj Thomsen  
Associate Professor

“The program can be used for determining the risk of scale formation as a function of temperature, pressure and composition. Output from the program includes the saturation index – showing the degree of saturation – which indicates the proximity to saturation,” explains Associate Professor Kaj Thomsen, CERE, lead developer of the program.

The software is also highly relevant to geothermal energy production.

“It is often necessary in geothermal energy production to dilute the brine before it is re-injected in order to avoid precipitation of salts in valves, pumps and the pores at the injection site. The amount of dilution required can be calculated with this program,” says Kaj Thomsen.

The thermodynamic model applied in the program is the Extended UNIQUAC model. The program can calculate solid-liquid equilibrium in aqueous systems with the ions  $\text{Na}^+$ ,  $\text{H}^+$ ,  $\text{Mg}^{2+}$ ,  $\text{Ca}^{2+}$ ,  $\text{Ba}^{2+}$ ,  $\text{Sr}^{2+}$ ,  $\text{Cl}^-$ ,  $\text{OH}^-$ ,  $\text{SO}_4^{2-}$ ,  $\text{HSO}_4^-$ ,  $\text{CO}_3^{2-}$ ,  $\text{HCO}_3^-$  up to high pressures.

The software is available to CERE industrial consortium partners free of charge.

## Strong software for carbon capture

Also building on the Extended UNIQUAC model is a CERE tool for carbon capture, the “CAPCO2”.



Philip I. Fosbøl  
Assistant Professor

“An energy corporation planning a  $\text{CO}_2$  capture unit can use the software for calculating the cost per volume of  $\text{CO}_2$  captured. Further, one can see how large the unit will need to be in order to capture the desired amount of  $\text{CO}_2$ ,” explains Assistant Professor Philip I. Fosbøl, lead developer of CAPCO2.

So far, CAPCO2 has been supplied to interested parties free of charge. However, as interest in carbon capture slowly but steadily increases in a number of countries, a commercial product might be considered.

“Benchmarking in the EU project Octavius has already shown CAPCO2 to be at least as accurate as the best programs available from other research groups, and we are gradually improving the software. For instance, we are currently extending the software to new promoted solvents containing piperazine,” says Philip I. Fosbøl, noting that the program is easy to use as it is Aspen Plus process simulation compatible.

“Processes for carbon capture are continuously being improved. When a company or a research group has a suggestion for a new process, CAPCO2 can calculate the energy consumption for the process.”

## Matlab compatible software coming up

The software portfolio of CERE will soon greet a new product.

“We have been inspired to create a new programming tool, which reinforces problem solving for chemical engineers,” says software manager Alay Arya.

The tool will build on a long-standing CERE success, the SPECS, which is a program that can present results from phase-equilibrium calculations as tabular formats and graphical plots, which can be obtained and understood without any need of programming skills. However, as is generally true for commercial graphical user interface software, the functionality of SPECS is limited.

“The coming tool – which yet has to be named – is a set of wrapped Fortran thermodynamic routines pro-compiled into a dynamic link library with a Matlab interface on top. It will implement a multi-component data base with a set of chemical properties. What is more, it integrates many thermodynamic models and algorithms so that it allows performing P-xy, T-xy, Phase-Envelope and many other calculations,” explains Alay Arya.

Matlab is a widely used engineering and programming language for numerical computation and visualization.

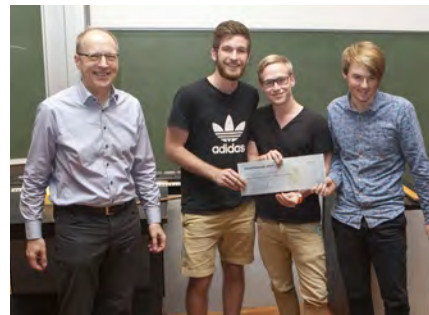
“Matlab makes problem solving and programming relatively easy for a chemical engineer without involving high programming skills. By integrating the coming tool in Matlab, the results can be further processed and shown in depth using other mathematical and plotting tools offered by that platform,” says Alay Arya. “Consequently, the new product will provide a more advanced approach to thermodynamic modelling as it is the chemical engineer who decides what functionalities his program or Matlab script will implement. In other words it opens the door to a wide range of new functionalities.”



# News from CERE

## Virtual Hunt for Oil

Close to 1,700 students from 32 high schools took part in the 2014 version of the Danish leg of the international PetroChallenge competition. CERE coordinates the event, which has been growing rapidly in popularity, each year setting new records for participation.



*Former CERE Chairman Erling H. Stenby presents the winning team with their prize.*

In the competition the students compete in teams at finding and producing oil in the simulation program OilSim, which is also used by the real oil and gas hunters in industry.

The winning team consisted of Alexander Victor Koefoed, Magnus Jørgensen and Jeppe Madsen, Svendborg Tekniske Gymnasium. Besides a cash prize the team won the right to represent Denmark at the international PetroChallenge finale in London 2015.

The prize was presented to the winners by former CERE Chairman Erling H. Stenby. Professor Stenby has been a leading figure in organizing the annual event since its introduction in Denmark in 2005.

Maersk Oil and DONG Energy sponsored the 2014 event.

## Leading Role for CERE in Bio-energy Research

A consortium of Danish research institutions and private companies has set out to create a platform for converting biomass into high-value energy resources. Technology for transforming agricultural waste products and similar types of biomass into “syn-gas” – a mixture of H<sub>2</sub>, CO and CO<sub>2</sub> – is already present. However, syn-gas is of limited use in itself and the new project will develop technology for converting the mixture into higher value energy products. For instance these could be ethanol – suitable as a fluid fuel – or methane of a quality ready for use in the natural gas distribution system.

The project is named Synferon (Optimised SYNgas FERmentation for biofuels production) and is planned for 3.5 years beginning by spring 2015. Of the total budget of 2.8 million EUR, 2.3 million EUR is financed by the Danish Innovation Fund, while the partners contribute with the remaining 0.5 million EUR. CERE Chairman, Professor Georgios Kontogeorgis will coordinate the project.

## Visit by a Geo-Thermal Energy Pioneer

Professor Seung Rae Lee of the Korean Advanced Institute of Science and Technology (KAIST) joined DTU as a visiting professor in 2014. The stay allowed him to engage in the geothermal energy storage activities at CERE led by Professor Ida L. Fabricius.

“Being a geologist, Ida focusses at rock structures at large depth, while I, as a geo-engineer, usually study clay and other types of soft soil near the surface. In geo-thermal energy storage we have found a field in which our competencies can be joined optimally,” says Professor Lee.

After obtaining his PhD at Stanford University, USA, Seung Rae Lee returned to KAIST in 1989, soon to become head of the institute’s group on geo-engineering.

“I guess you can say that I have become a pioneer in geo-thermal energy. The typical geo-thermal practitioner would be either a mechanical engineer or a civil engineer specializing in buildings. Both groups tend to overlook the importance of the local geology when designing a geo-thermal system.”

Using a combination of commercially available software and original software developed in his group at KAIST, Professor Lee hopes to be able to simulate easily and accurately what would be the required geo-thermal design for a given location.

The stay at DTU was part of a one-year sabbatical, which also included a stay at the Technical University of Munich (TUM).

## CERE Professor receives Chemical Engineering Award

Professor Michael L. Michelsen, CERE, was awarded the 2014 EFCE Distinguished Lecture in Thermodynamics and Transport Properties by the European Federation of Chemical Engineering.

Professor Michelsen was given the award in recognition of his long and outstanding career in applied thermodynamics, especially the development of rigorous algorithms for multicomponent, multiphase equilibria, and thermodynamic models suitable for practical applications e.g. in the chemical and petroleum industries.



*Michael L. Michelsen, Professor.*

The award was given for the second time. The first receiver was Dr. Andreas Klamt in 2012.



Find out when the next Advanced Course takes place

## Danish Hydrocarbon Research Center Established

By September 2014, the Danish Hydrocarbon Research and Technology Centre opened at DTU. The new center is a close partner to CERE. Its purpose is to develop new knowledge, ideas and methods for increasing the extraction of oil and gas in the North Sea.

“The perspective inherent in pursuing studies in the field of oil and gas is that it gives young people direct access to an industry that is big, important and among the most knowledge and energy-intensive in the world. As the area is constantly developing, we will need people skilled in this field for many years to come,” Bo Cerup-Simonsen, Director of the center, said at the inauguration.

The new center is backed by the Danish Underground Consortium (DUC), which consists of A. P. Møller – Mærsk (31.2 %), Shell (36.8 %), Chevron (12 %), and the state-owned Nordsøfonden foundation (20 %).

The activities will involve close interaction between academia and industry. “In the oil and gas industry, we have a pressing need for new solutions to improve the efficiency of extraction. There is still a lot of potential in the Danish section of the North Sea, but it is becoming more and more difficult to extract the oil. That is why we will need new knowledge and technology far into the future. Gaining a university degree in the area of oil and gas is a ticket to an international high-tech industry, and graduates will be able to help identify solutions of huge benefit to society,” said Troels Albrechtsen, Chairman of the DUC Operating Committee.

## Honored for Greenhouse Gas Reviewing

Certificate of Excellence in Reviewing was awarded to Associate Professor Kaj Thomsen, CERE, in recognition of an outstanding contribution to the quality of the International Journal of Greenhouse Gas Control 2013.



### A busy Year for the Petroleum Engineers of Tomorrow

For several years now has the DTU Student Chapter of the Copenhagen section of the Society of Petroleum Engineers (SPE) grown steadily. In 2014, the number of members reached 110. The high level of memberships was matched by an impressive level of activity throughout the year.

By March, the chapter and CERE Associate Professor Alexander Shapiro organized a guest lecture by Son Huu Do of 3Dos Global Energy, San Diego, USA, on enhanced oil recovery. The lecture was attended by 65 Master and PhD students.

Later the same month, Maersk Oil hosted 20 chapter members. Dr. Vural Sander Suicmez, senior reservoir engineer at Maersk, challenged the students to a team competition in which they were to solve a case study from practical reservoir engineering. Further, Lee Milligan of the Maersk Oil recruitment program for graduates, and Hans Horikx, the company's Chief Reservoir Engineer, introduced the various career opportunities in Maersk.

Another 18 students from the chapter were invited to visit Schlumberger's facilities in Esbjerg. The visit was hosted by Børge Mathiesen from the company. The presentations covered Schlumberger's activities in general, and coil tubing, wireline and logging tools, and well testing in more detail. The field trip also included a visit at the M-I SWACO/D&M office with Søren Brink Jensen as host.

Two DTU master students, Birgit Haastrup and Leonardo Meireles, took part in the SPE European Regional Student Paper Contest. Held in June at the Imperial College, London, the competition saw abstracts in three different categories – Bachelor, Master, and Doctorate. Birgit Haastrup won the master category for her project on “Enzyme penetration tests on chalk cores”, while Leonardo Meireles took third place in the same category for his study on “Effect of

divalent ions on solid-fluid interface, as observed by NMR transverse relaxation time”.

Last but not least, the DTU Student Chapter and Alexander Shapiro, CERE, hosted a large event by September 2014, introducing around 75 DTU bachelor students to the petroleum engineering education. Hans Horikx, Maersk Oil, chairman of the SPE Copenhagen section, appeared as guest speaker, while Bo Cerup-Simonsen, Director at the Danish Hydrocarbon Research and Technology Centre, introduced the scope of the new center.

### Maersk Oil takes CERE to the Movies



*Postdoc Sidsel Marie Nielsen is one of the CERE researchers to appear in the movie on BioRec.*

The BioRec project (Biotechnology in Oil Recovery), coordinated by CERE, features in a short movie produced by Maersk Oil. The movie is part of a series on how the company, one of the partners in BioRec, contributes to the Danish society in various ways. The movie can be found at the company's website.

### Greek Guest contributes on Molecular Thermodynamics

Through a 3-month Visiting Professor stay, Professor Costas G. Panayiotou, Aristotle University of Thessaloniki, Greece, brought new input to the Department of Chemical Engineering DTU. His main interest is molecular thermodynamics, which is a combination of quantum mechanics, statistical mechanics and chemical thermo-dynamics. During his

stay, Professor Panayiotou mainly cooperated with two centers at the department, namely CERE and CAPEC-PROCESS.

“Both centres are interested in powerful predictive tools. The stay here has given us the opportunity to explore how tools from my field of expertise, which is molecular thermodynamics of bio-polymeric systems, can be used by DTU and vice versa,” says Costas G. Panayiotou.

During his stay, Professor Panayiotou gave several lectures and seminars, all well attended by CERE staff, members of the CERE industrial Consortium, and by PhD students. He also participated in the CERE Discussion Meeting 2014, where he had the opportunity of discussing possible future collaboration between his own institution and DTU with possible involvement of CERE partners.

“A number of research areas have been identified as potential areas of collaboration with industrial participation. This may involve our complementary expertise on modelling highly complex systems over a broad range of external conditions of temperature, pressure, and composition,” Professor Panayiotou states.

The scientific part of his stay included research on a novel approach for characterization of solid surfaces, especially determination of surface energy and surface tension of polymer surfaces.

The stay was made possible by a grant from the Otto Mønstedts Foundation.

### US and Norwegian Input on Petroleum Engineering

The University of Wyoming has established a strong experimental facility within petroleum engineering. In April 2014, Dr. Mohammad Piri of the American university visited CERE and gave a seminar. He outlined the general scope of the facility, which provides unique opportunities for

studying reservoir conditions, three-phase flow, and computed tomography. Further, Dr. Piri presented results from experiments on the effect of saturation history on three-phase relative permeability.

Similarly, the Norwegian University of Science and Technology in Trondheim has established a Center for Integrated Operations in the Petroleum Industry. In August 2014, Professor Bjarne Foss visited CERE to introduce the Integrated Operations Center, and also to give a seminar on both long-term and short-term optimization of oil production. His presentation highlighted the value of integrating petroleum engineering with systems control engineering groups.

### Advanced Course on Thermodynamic Modelling



*29 participants of 11 different nationalities took part in this years' course.*

The tradition was kept alive, as CERE offered its annual “Advanced Course on Thermodynamic Models”, January 6-17, 2014. Like previous years, the course was fully booked. The 29 participants were of 11 different nationalities. Four private companies were represented, as well as

11 foreign academic institutions, and also a number of CERE PhD students.

The course supplied an overview of the most important thermodynamic models used in industrial practice, including how efficient computer codes for such models are written and checked for errors. During the practical part of the course, participants would develop their own codes.

The models in use included equation of state and activity coefficient models, EoS/GE mixing rules, association models (the CPA and SAFT equations of state), mixtures with electrolytes and polymers, applications including Carbon Capture and Storage as well as flow assurance and trends in thermodynamic models.

Also in accordance with a fine tradition, the course was chaired by CERE Professor Michael L. Michelsen.

### Gearing up for Deep Oil Exploration

Plans by several energy corporations to pursue oil and gas exploration at large depths are accompanied by the purchase of advanced equipment at CERE. The new PVT apparatus (pressure, volume, temperature) can study reservoir fluids at high pressure, high temperature (HPHT) conditions present in exploration at large depth. The apparatus consists of units for fluid recombination, PVT measurement, high pressure viscosity measurement, and asphaltene precipitation studies. All units can be operated up to 1,500 bars and 200 C. Equipped with a high pressure sapphire window, the PVT cell in the apparatus allows full visual observation of phase change at HPHT. The apparatus is purchased as a part of the NextOil project coordinated by CERE and funded by the Danish National Advanced Technology Foundation (today Innovation Fund Denmark).



Read more at our website



# Petrophysics of Palaeogene Sediments



Ahmed Awadalkarim, PhD.

Full title: “Petrophysics of Palaeogene Sediments”.

Supervisor: Ida L. Fabricius.

Funding: DTU.

Almost all of the world's oil fields are situated in sedimentary rock. The chalk of the North Sea is one example. Permeability, strength, and other physical properties of the buried sediments are important to hydrocarbon exploration. The properties of the buried sediments are highly variable and controlled by factors such as mineralogical composition, depositional texture, and burial depth.

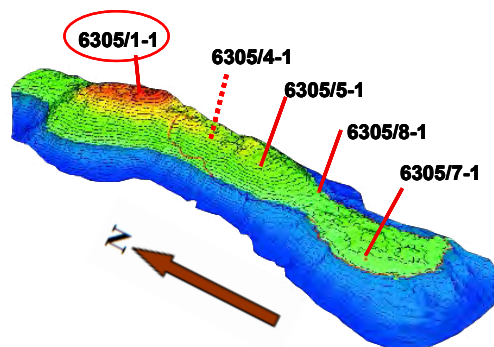
The thesis investigates Palaeogene sediments, which are relevant to oil exploration. How properties vary with burial depth is given special focus.

Three lithologies were selected for study: the Eocene chalk of the Atlantic Ocean; the siliceous ooze sediments from the Norwegian Sea; and the Palaeogene shale from both the Atlantic Ocean and the Danish Basin. The three geological settings differ in water depth, temperature, effective stress, and pressure. An improved understanding of the factors governing the physical properties of the sediments with these lithologies will benefit the petroleum industry. For instance, drilling

through intervals of shale or siliceous ooze sediments could result in severe and very costly borehole instability problems related to the properties of shale.

The effective stress is a key factor when trying to predict the geo-mechanical behavior of shale. Biot's coefficient ( $\beta$ ) is an indicator for sediment stiffness which is a property of sediment structure. Engineers have generally assumed  $\beta$  equal to one when estimating in-situ vertical effective stress on buried sediments. However, this assumption is not always right. Especially for the deep-sea sediments where the water depth is high, the real effective stress can be underestimated. This may again lead to severe engineering consequences such as a petroleum reservoir suffering from compaction or deformations during drilling operations and hydrocarbon production.

In the project changes in physical properties of the Atlantic Palaeogene shale as a function of burial depth were related to the vertical effective stress and shale mineralogy. The influence of choice of  $\beta$  value on estimation of effective stress on deep-sea shale was shown.



Further, the changes of porosity and sonic velocity trends of Eocene chalk were related to effective stress and the time-temperature index of thermal maturity of chalk. It is concluded that the use of Biot's effective stress concept provides more realistic estimates of vertical effective stress.

The study includes a study on siliceous ooze in the Norwegian Sea. A new approach for deriving reliable porosity estimates for siliceous ooze is proposed.

Finally, X-ray diffraction (XRD) analyses and surface area calculations by the BET method were done on 116 sediment samples from different geological units in the Fehmarn Belt. Based on the results, ten whole-core samples of Palaeogene clay were selected for elastic deformation studies. Mineralogy, BET, classification parameters, elastic wave velocities, and strain caused by mechanical loading were measured. The obtained results can be used for estimation of geotechnical drained elastic modulus from bulk density and elastic wave velocity. This may again aid engineering practice, including structural design and slope stability analysis.



Location map of the Ormen Lange gas Field (right), not to the scale. The five wells included here are shown to the left figure on the North-South trending doubly plunging anticline with two structural highs.

# Modelling the Behavior of Mixtures with Electrolytes



Bjørn Maribo-Mogensen, PhD.  
Currently Linde, Germany.

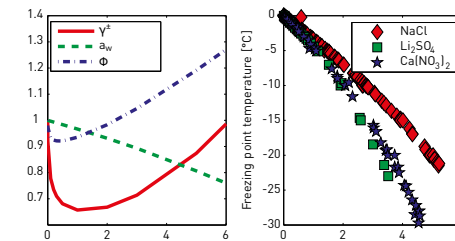
Full title: “Development of an Electrolyte CPA Equation of state for Applications in the Petroleum and Chemical Industries.”

Supervisors:  
Georgios Kontogeorgis, Kaj Thomsen.

The project was funded by the Joint Industry Project CHIGP (2/3) and DTU (1/3).

Presence of salts in oil and gas recovery tends to cause a salting out of hydrocarbons from the brine. Furthermore, the presence of electrolytes may enhance the effect of methanol and glycol which are added to inhibit formation of gas hydrates in natural gas pipelines. Therefore it is essential for the oil and gas industry to be able to model the behaviour of mixtures containing electrolytes. This is even more relevant now, as operations are extended to deep reservoirs with high pressure, and high temperature (HPHT). Generally, modelling is highly important in HPHT due to scarcity of experimental data, and specifically, a better understanding of electrolyte solutions is crucial for predicting operation limits and establishing adequate safety measures. The topic is also relevant to the chemical industry and other industries.

In the thesis an equation of state (EoS) capable of handling mixtures containing electrolytes is presented. The model is named e-CPA, where the “e” is for electrolyte, and CPA is the Cubic Plus Association EoS, which has been applied to a wide range of industrially important chemicals over the last 18 years.



Effect of NaCl concentration at 25° C on mean ionic activity coefficient  $\gamma_{\pm}$ , water activity  $a_w$ , and osmotic coefficient  $\Phi$  (left) [2]. Effect of different salts on the freezing point of water as a consequence of the reduced water activity (right) [13].

During the project the e-CPA was applied to a number of contexts.

Firstly, the solubility of light gases, hydrocarbons, and aromatics in aqueous mixtures and mixed solvents was predicted.

Secondly, the model proved capable of predicting solid-liquid equilibrium in aqueous salt mixtures and mixed solvents.

Thirdly, gas hydrate formation pressures of methane with salts in water + methanol were predicted.

And finally, liquid-liquid and liquid-liquid-liquid equilibrium with water-propan-1-ol-NaCl-octane solutions was calculated.

It was demonstrated that the model has a good potential for application in relation to e.g. flow assurance during the production of natural gas.

A further advantage of the model is the fact that it reduces to the CPA EoS in the absence of electrolytes, making it possible to extend the applicability of the CPA EoS while retaining backwards compatibility and re-using the parameters for non-electrolyte systems.

The work meets a long-standing industrial need for a better tool for modelling the behaviour of mixtures containing electrolytes. A recent survey by the European Federation of Chemical Engineers (EFCE) revealed that:

“The predictive capabilities of thermodynamic models for electrolyte mixtures lag years behind their non-electrolyte counterparts and there is an industry-wide consensus that new predictive (rather than correlative) models are strongly needed.”

The work contributes to the understanding of the behaviour of mixtures containing electrolytes. The static permittivity of a mixture was found to be the most important property. Thus, a new theoretical model was developed to extend the framework for modelling the static permittivity to hydrogen-bonding compounds and salts. The model relates the geometrical configuration of hydrogen-bonding dipolar molecules to the Kirkwood g-factor using the Wertheim association model that is included with modern EoS such as CPA or SAFT (Statistical Associating Fluid Theory). The new model was shown to give excellent predictions of the static permittivity of mixtures over wide ranges of temperature, pressure, and composition.

Further, the CPA EoS was extended with a Debye-Hückel and a Born term to account for the electrostatics along with the new model for the static permittivity. The new e-CPA EoS was parameterized against osmotic coefficient, density, and mean ionic activity coefficient data and validated against salt mixture data.



# Stability of Danish CO<sub>2</sub> Storage Reservoirs



*Ernest Ncha Mbia, PhD.  
Currently Postdoc,  
University of Calgary, Canada.*

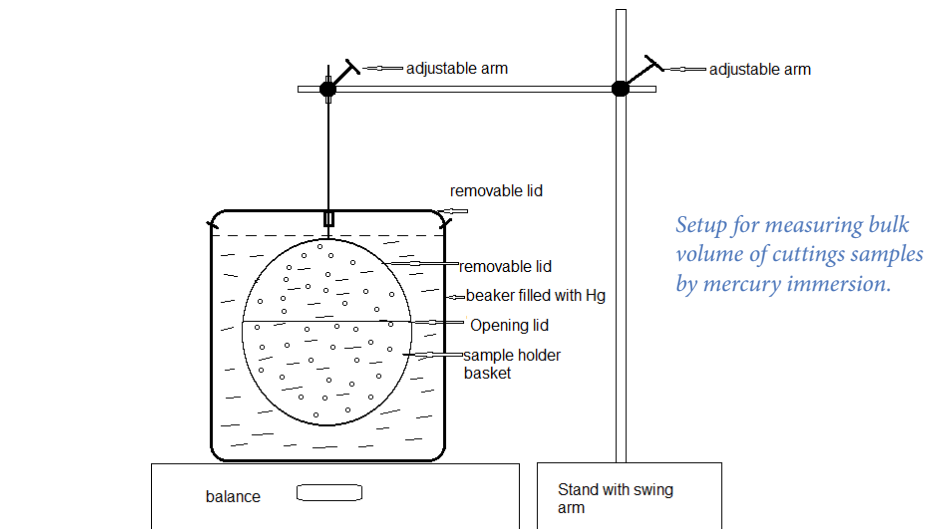
*Full title: "Assessment of Dynamic Flow, Pressure and Geomechanical Behavior of a CO<sub>2</sub> Storage Complex".*

*Supervisors: Ida L. Fabricius, Peter Frykman (GEUS), Finn Dalhoff (Vattenfall).*

*The project was funded by the Danish Strategic Research Council, and Vattenfall.*

The increasing CO<sub>2</sub>-level in Earth's atmosphere is a major concern to society. A number of countries carry out CCS projects (Carbon Capture and Storage) that aim at limiting the release of the primary greenhouse gas, carbon dioxide (CO<sub>2</sub>), in order to mitigate climate change. Several CCS projects aim at capturing CO<sub>2</sub> from coal fired power plants and storing it in suitable geological structures. If CCS is to play a role in climate protection, the projects will need to store large amounts of CO<sub>2</sub>.

The thesis addresses how the storage of large amounts of CO<sub>2</sub> will influence the stability of a geological structure that has been suggested as suitable for the purpose in Denmark.



Deep saline aquifers offer the largest CO<sub>2</sub> storage potential of all geological options. However, storing extremely large amounts of CO<sub>2</sub> could introduce additional fluids in the formation that may cause pressure changes and displacement of natural brines. If this happens it will be of great environmental concern especially to the ground water and other subsurface resources. Even if the injected CO<sub>2</sub> is safely trapped in suitable geological structures, pressure changes and brine displacement may affect shallow ground water resources, for example by increasing the rate of discharge into a lake or a stream, or by mixing brine into drinking water aquifers.

The Vedsted structure in Northern Jutland has been considered for CO<sub>2</sub> storage. The primary cap-rock is the 530 m thick Fjerritslev Formation sealing the Gassum Formation. Samples from deep wells both in Vedsted and Stenlille (Sjælland) were studied and compared to samples from Skjold Flank in the North Sea. The samples were analyzed by X-ray diffraction (XRD) in order to establish mineral composition and pore sizes.

It was demonstrated that elastic moduli as calculated from bulk density and velocity of elastic waves relate to equivalent pore radius of studied shales. This relationship establishes the possibility of calculating equivalent pore radius from logging data.

In a second part of the project a simulated CO<sub>2</sub> storage scenario in the Vedsted structure was considered. In the scenario 60 million tons of CO<sub>2</sub> was injected at a rate of 1.5 Mt/year into the underlying Gassum Formation over 40 years. The sensitivity of cap-rock permeability and compressibility towards pressure development and transmission to the shallower Chalk Group (where the brine-fresh water interface resides) was assessed. The results indicate that an overpressure difference of about 5 bar is created in the reservoir.

Seismic profiling of the structure shows the presence of faults. In order to evaluate potential risks associated with vertical pressure transmission via the faults through the cap-rock, simulations of both worst and best case scenarios have been undertaken. The results show that in the worst case, the overpressure of 5 bar is transmitted to the Chalk Group, while in the best case the overpressure is confined within the primary cap-rock.

Overall, the results based on both best and worst case scenarios show no potential threat to CO<sub>2</sub> storage in the Vedsted site. The work underscores the importance of obtaining site specific data for simulation studies of potential CO<sub>2</sub> storage sites.

# Heat Storage in Sandstone Aquifers



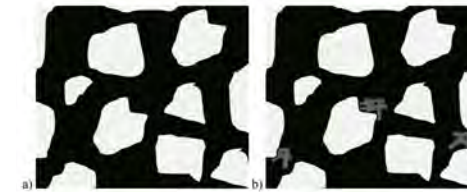
*Esther Rosenbrand, PhD.  
Currently Royal Haskoning DHV,  
The Netherlands.*

*Full title: "Effect of Temperature on Sandstone Permeability."*

*Supervisors: Ida L. Fabricius, Claus Kjeller (GEUS).*

*The work is a part of the Heat Storage in Hot Aquifers project (HeHo), which is a research collaboration including DTU, GEUS, the University of Vilnius, and Dansk Fjernvarmes Geotermiselskab. Funding is provided by the Danish Council for Strategic Research.*

Geo-thermal energy is used for district heating in Copenhagen and Thisted, and several other Danish cities are considering the establishment of new facilities. Whereas heat is produced all year long, the demand for heat peaks in winter. This has spurred interest in seasonal heat storage. It has been suggested that heat can be stored in deep, warm aquifers with relatively small losses. However, one has to pay attention to the effect, which the method might have on the permeability of the rock



*Schematic representation of sandstone consisting of framework grains (white) and pores (black). b) Schematic representation of sandstone containing clay particles (grey) in some intergranular pores (pores among framework grains). Smaller pores are also present among clay mineral particles.*

in question. If for some reason the injection of warm water was to decrease permeability, this would increase the energy demand for injecting and later extracting geo-thermal brine, thus inducing further costs and damaging the economic feasibility.

The thesis investigates how heat storage can be expected to influence permeability of sandstone. It has been suggested that sandstone aquifers will be the best practical solution for heat storage in Denmark.

The work is based on a combination of extensive literature studies and new flow-through experiments on Berea sandstone (which is often used as a reference material to reservoir sandstones) and on Danish Gassum Formation sandstone, and Bunter sandstone. Polished thin sections were studied by electron microscopy in order to relate permeability to sandstone texture.

An effective specific surface area per pore volume was estimated by using image analysis and pore size distributions from nuclear magnetic resonance (NMR) transverse relaxation data. The smaller pores in the pore size distributions appear to control permeability in sandstones with a low clay-free inter-granular porosity. Presumably in those sandstones larger inter-granular pores are only connected through smaller pores, which therefore limit

the flow rate in larger pores. In sandstones where larger inter-granular pores do form a connected flow path, the higher permeability in these pores would have the dominant effect on the measured permeability, wherefore the effective specific surface reflects the specific surface of the framework grains.

Both heating and reduction of the salinity of the pore fluid can increase the double layer repulsion between quartz grains and kaolinite particles in Berea sandstone, which could lead to kaolinite mobilization and permeability reduction. Heating increases the magnitude of the mineral surface charge, whereas salinity reduction increases the range over which the surface charge acts.

Flow-through experiments in Berea sandstone samples indicated differences between the effect of temperature and salinity on permeability. A permeability reduction at 20°C due to salinity reduction was not reversed by restoring the salinity. However, a permeability reduction due to heating to 80°C was reversible by restoring the temperature to 20°C. Therefore, it is suggested that mobilized kaolinite particles affect permeability by a different mechanism at 80°C than at 20°C. At 80°C the main effect might be due to an alteration of pore fluid rheology, whereas at 20°C particles might be filtered in pore constrictions.

Kaolinite is observed in samples of Gassum Formation sandstone from different localities. To avoid permeability reduction by hot water injection, localities with low kaolinite content would be preferred. If, however, hot water injection is planned in localities with high kaolinite content, effects of flow rate and temperature on permeability can be investigated by means of additional flow-through experiments, using the in-situ pore fluid composition and the range of flow rates that would be expected in the aquifer.



# Advanced Amine based Carbon Capture



Muhammad Waseem Arshad, PhD.  
Currently Postdoc, CERE.

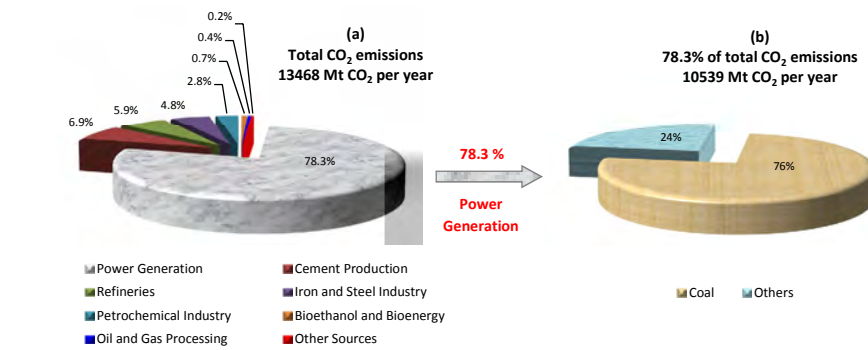
Full title: “Measuring and Thermodynamic Modeling of De-mixing CO<sub>2</sub> Capture Systems”.

Supervisors: Kaj Thomsen, Nicolas von Solms.

The project was financially supported by the European Commission within the iCap project (Innovative CO<sub>2</sub> Capture) under the 7th Framework Program.

Carbon Capture and Storage (CCS) has been suggested as one of the solutions for mitigating climate change caused by anthropogenic emissions of CO<sub>2</sub>. Amine based carbon capture is a mature and commercially available technology, with monoethanolamine (MEA) being a very well-studied solvent. However, the MEA process is energy intensive, which adds to costs.

The thesis presents a de-mixing solvent system consisting of two amines, 2-(diethylamino) ethanol (DEEA) and 3-(methylamino)propylamine (MAPA). The proposed system has a potential for reducing the energy penalty of the capture process.



A profile of stationary point sources emitting more than 0.1 Mt CO<sub>2</sub> per year. a, CO<sub>2</sub> emissions in percentage of different sources for the total CO<sub>2</sub> emissions of 13468 Mt per year; and b, CO<sub>2</sub> emission contributions from coal and other fuels (natural gas, fuel oil, and other fuels) to the 78,3 emissions (10539 Mt CO<sub>2</sub> per year) from power generation.

DEEA is a tertiary alkanolamine and MAPA has two amine functional groups, a primary and a secondary. Both have certain qualities for carbon capture, but are not ideal for the purpose. A blend of DEEA and MAPA exploits the favorable properties of both.

Further, when a mixture of DEEA and MAPA at certain concentrations reacts with CO<sub>2</sub>, it forms a biphasic liquid-liquid phase change (de-mixing) giving an upper liquid phase lean in CO<sub>2</sub> and a lower liquid phase rich in CO<sub>2</sub>. The CO<sub>2</sub> lean phase is sent back to the absorber without regeneration and only the CO<sub>2</sub> rich phase is sent to the stripper for regeneration. Due to a low liquid circulation rate in the stripper, one can reduce the solvent regeneration energy.

In the project freezing point depression measurements were performed for binary aqueous DEEA and MAPA solutions at different concentrations of amine and for the ternary DEEA-MAPA aqueous solutions for different molar ratios. The data were compared with MEA and methyl diethanolamine (MDEA) as references. The results indicate that the non-ideal behavior of DEEA is almost similar to that of MEA. However, MAPA shows a stronger non-ideal behavior compared to DEEA and MEA.

Differential heat of absorption of CO<sub>2</sub> in DEEA, MAPA, and mixtures of the two were measured at different temperatures (40, 80, and 120 °C) and CO<sub>2</sub> loadings. The data was compared with 30 mass % MEA as reference.

5 M DEEA showed a high CO<sub>2</sub> loading capacity at 40 °C and a very low loading capacity at 120 °C, thus giving a high CO<sub>2</sub> cyclic capacity. Both 2 M and 1 M MAPA showed high loading capacities at both 40 °C and 120 °C, thus giving a relatively lower capacity.

Thermodynamic modelling of the de-mixing system and the two sub-systems, H<sub>2</sub>O-DEEA-CO<sub>2</sub> and H<sub>2</sub>O-MAPA-CO<sub>2</sub>, was performed by Extended UNIQUAC. 100 model parameters and thermodynamic properties were fitted to over 1,500 experimental data consisting of pure amine vapor pressure, vapor-liquid equilibrium, solid-liquid equilibrium, liquid-liquid equilibrium, excess enthalpy, and heat of absorption of CO<sub>2</sub> in aqueous amine solutions. With a single unique set of parameters, the developed model can reproduce almost all the binary, ternary, and quaternary data points and can describe all data types for the studied systems satisfactorily.

# A Smooth Method for History Matching



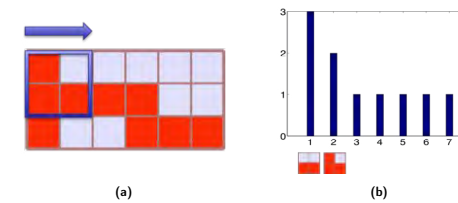
Yulia Melnikova, PhD.

Full title: “Solving Inverse Problems through a Smooth Formulation of Multiple-Point Geo-Statistics”.

Supervisors: Klaus Mosegaard, Alexander Shapiro, Erling H. Stenby.

Funding: the Danish Council for Strategic Research, and DONG Energy.

Currently, Denmark is missing out on more than 70 % of its North Sea oil, which is trapped in unreachable parts of the reservoirs. Improving the rate of recovery is highly desirable. Accurate reservoir description plays a key role to problems associated with recovery of hydrocarbons, risk estimation, and predicting reservoir performance. Reservoir characterization uses seismic surveys, well logs, production data, geological maps, and other sources of data, expertise and numerical methods in order to describe subsurface structures, locations of fluids and properties of rock. Much like in astrophysics where we cannot observe the interior of the stars directly, geoscience uses indirect observations in order to obtain information about an



Example of a binary discrete image (a) and its frequency distribution for a 2X2 template (b)

unknown system. This is done by means of solving inverse problems. While a direct problem is calculating the signals – for instance sound or electromagnetic waves – by known parameters of the subsurface, an inverse problem is reconstructing these parameters by measured signals. The thesis introduces a solution to inverse problems related to oil and gas exploration through a smooth formulation of multiple-point geo-statistics.

The main motivation for the study is the challenge posed by history matching, which is an inverse problem aimed at estimating rock properties from production data. History matching faces two main difficulties, which are the existence of multiple often geologically unfeasible solutions, and high computational cost of the forward simulation.

In the project a new method for solving inverse problems is developed. Importantly, the method focusses on limiting the demand for computational time, which makes it attractive for practical implementation.

The method is inspired by the Frequency Matching method developed by the group earlier. Both methods build on quantifications of the probabilities of various parameter estimations, recognizing that uncertainty will exist. Further, both methods include complex a priori information in order to exclude solutions that are geologically unacceptable. Such in priori information may be inferred from a conceptual geological model termed a “training image”.

In the smooth formulation method, data and multiple-point statistics are integrated in a framework which allows a solution to be found by use of gradient-based optimization. As a result, solutions to inverse problems are obtained efficiently by deterministic search.

Both the smooth formulation and the Frequency Matching method find the solution by maximizing its posterior probability. This is achieved by introducing a closed form expression for the a priori probability density. We have defined an expression for the training-image based prior by applying the theory of multinomial distributions. Its combination with the likelihood function results in the closed form expression for defining relative posterior probabilities of the solutions.

Finally, the developed smooth formulation was applied to the problem of seismic inversion. The proposed methodology allows inversion of seismic reflection data for rock properties, namely for porosity, by integrating rock physics models into the inversion procedure. Errors associated with conversion from depth to time are handled with a novel mapping approach.

In conclusion, the proposed method offers a balance between consistent data integration and computational costs and can be seen as an efficient, probabilistically formulated optimization scheme for solving inverse problems. The applicability to problems of history matching and seismic inversion is demonstrated, and the method has a potential to be applied in practical reservoir management.



# A Systematic Approach to Chemical Product Innovation



Michele Mattei, PhD.  
Currently Akzo Nobel, The Netherlands.

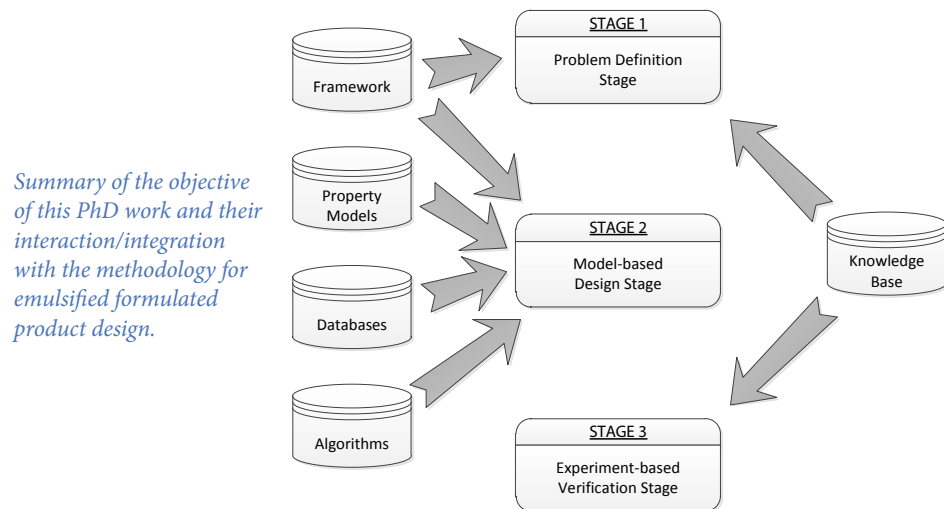
Full title:  
“Advances in Chemical Product Design”.

Supervisors:  
Rafiqul Gani, Georgios Kontogeorgis.

Funding: DTU, CAPEC-Process, CERE.

Chemical household products like hand-wash soap, sun lotion etc. are mainly designed by “trial-and-error” based techniques. This thesis proposes an alternative, systematic approach to chemical product design. Such approaches have been applied with success in other engineering fields.

The project focusses on emulsified formulated products. Emulsions are defined as mixtures of two normally immiscible liquids, kinetically stabilized by the so-called emulsifying agents that lie at the interface between the two liquid phases.



Most often surface active agents, surfactants, are used as emulsifying agents. Active ingredients and additives are then dissolved in the continuous and/or in the dispersed phases. Emulsified products are found in a vast number of household products, for instance in many food and cosmetic products.

In this work a systematic approach for the design of emulsified formulated products is proposed and applied to three test studies, consisting of a UV sunscreen, a tank-cleaning detergent, and a hand-wash soap.

The methodology consists of three integrated stages: a problem definition stage where consumer needs are converted into quantitative information; a model-based stage where property models, structured databases, and dedicated algorithms are integrated in order to propose a candidate formulated product; and finally an experiment-based stage for validation and refinement aimed at reaching the final emulsified formulation.

Each of the three stages is divided into tasks with several sub-tasks. Systematic data-flow and workflow link the different sub-tasks, generating a methodology which leads to the final product recipe.

For some sub-tasks the necessary models could be retrieved from the literature, while for others they had to be developed. For

instance, a step-by-step algorithm for design of solvent mixtures in the emulsified form (EMUD) was developed in the project, and integrated with another algorithm previously developed for design of homogeneous formulations, forming a robust tool for mixture design.

Databases of both active ingredients and additives have been built, including properties of relevance to the design procedure. Moreover, a knowledge-base has been developed for the problem defining stage. The overall workflow, models, methods, and tools have been integrated as a new template into an in-house software, the virtual Product-Process Design Laboratory, for the design and analysis of emulsified formulated products.

Finally, the methodology was tested in three case studies. For one of them, a hand-wash soap, the whole methodology was applied, including manufacture of a final prototype. For the other two, a UV sunscreen and a tank-cleaning detergent, both the problem-defining stage and the model-based stage were conducted fully, while the experimental stage was partly performed.

The results confirm that the integrated methodology can be successfully implemented for screening thousands of alternatives, and for the generation of a short-list of promising candidates.

# Monitoring of Oil Spills at Sea



Xiaodong Liang, PhD.  
Currently Postdoc, CERE.

Full title:  
“Thermodynamic Modelling of Complex Systems”.

Supervisors:  
Georgios Kontogeorgis, Kaj Thomsen, Wei Yan.

The project was funded by the Danish National Advanced Technology Foundation (today the Danish Innovation Fund), and the Department of Chemical and Biochemical Engineering, DTU.

The accidents in the Gulf of Mexico in 1979 and 2010 caused two of the biggest oil spill disasters in history. Environmental safety is a major challenge to the oil and gas industry, especially as the offshore sector will continue to grow, while exploration and production will take place at ever more remote locations and at large depth. Locating spilled oil in the water by sonar detection is an important tool in reducing the environmental effects of offshore oil exploration. The thesis aims to contribute to the improvement of the quality of sonar detection by developing new and evaluating existing theory used for interpretation of monitoring results.

Sonar investigation can potentially detect oil and gas leaks around the sub-sea well head. This will enable faster responses, especially in deep water and in ice covered areas. Further, the method can map oil in the seawater column during the clean-up process after an oil spill. However, there is a need for better theoretical understanding of the method.

The oil spills in the Gulf of Mexico have shown that, contrary to earlier theories, the oil is not only present at the surface, but also in great volumes both in the water column and on the seafloor. This indicates that we do not know enough about how oil behaves in water. Moreover, modern oil recovery depends on significant amounts of gas hydrate inhibitors and other chemicals, which greatly increases the complexity of the investigation.

The classical thermodynamic models used by the oil industry are semi-empirical and not suitable for mixtures containing water and other polar compounds. Instead, the project builds on the Perturbed-Chain Statistical Association Fluid Theory (PC-SAFT) equation of state (EOS).

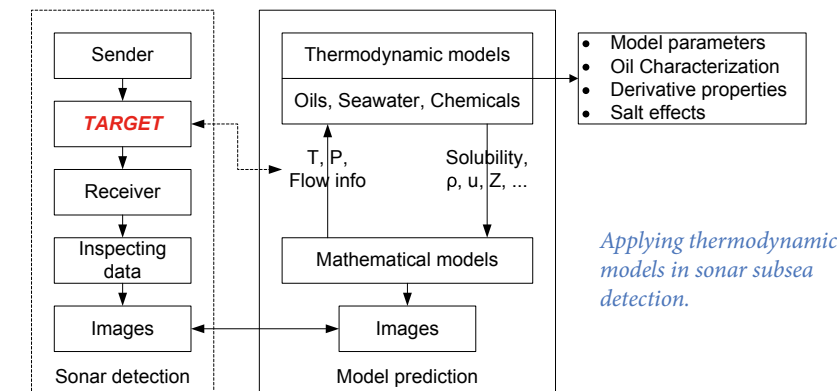
Firstly, the PC-SAFT EOS was successfully applied to model the phase behaviour of water, chemical and oil containing systems with newly developed pure component parameters for water and chemicals and characterization

procedures for petroleum fluids. An interactive step-wise procedure is proposed to fit the model parameters for small associating fluids by taking the liquid-liquid equilibrium into account.

Secondly, data for the speed of sound were reviewed. It is proposed to improve the description of speed of sound within the PC-SAFT framework by adding speed of sound data to the parameter estimation and/or the universal constant regression. The first approach works only for short associating fluids, while the second approach significantly improves the speed of sound description for various systems

Thirdly, the fundamentals of PC-SAFT were investigated based on universal constant regression. A new variant of universal constants has been developed, which avoids having more than three volume roots and an additional unrealistic critical temperature. It is shown that it is possible to use the original PC-SAFT parameters with the new universal constants directly for the systems considered in the project.

Overall, the project has contributed to enhancing the performance of sonar investigation for application in detection and monitoring of oil spills at sea.

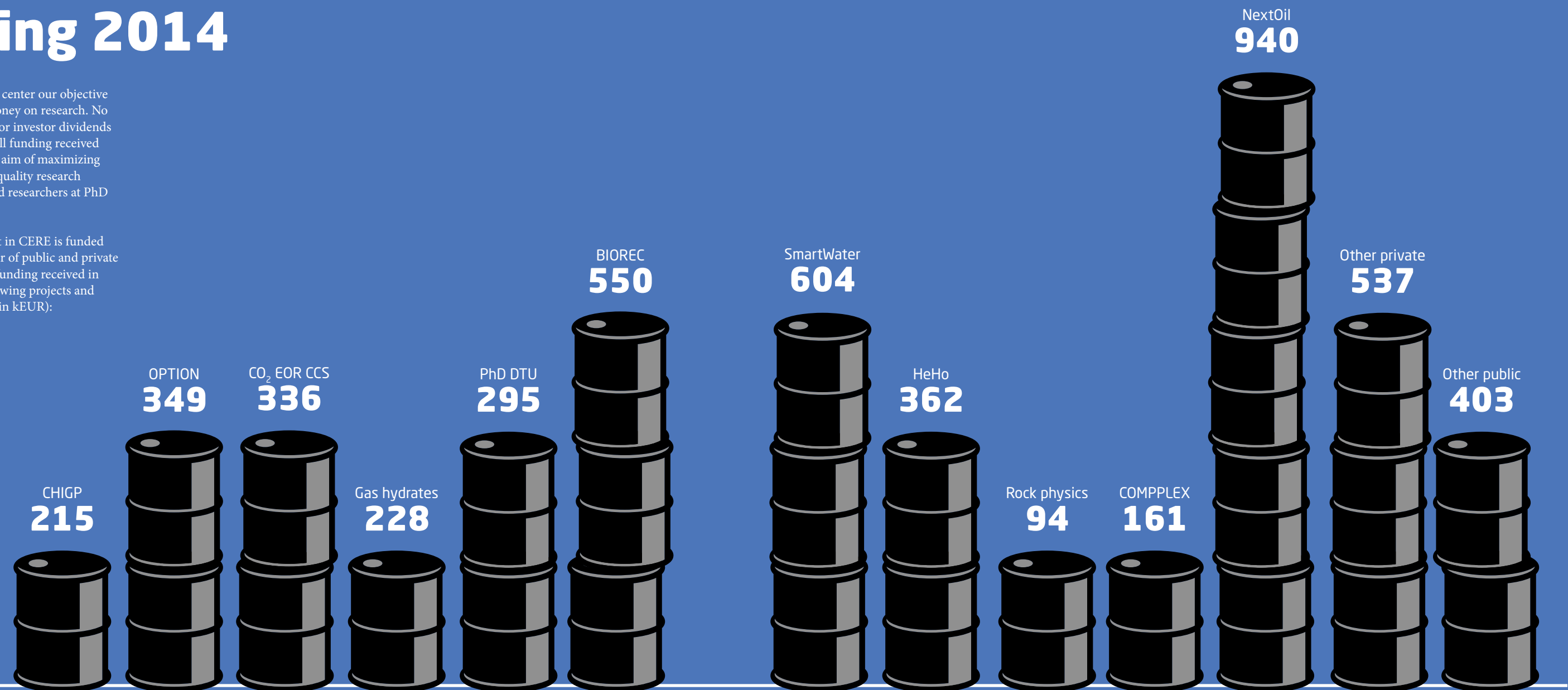




# Research Funding 2014

As a university research center our objective is to spend all of our money on research. No management bonuses nor investor dividends are due, and gradually all funding received will be invested with the aim of maximizing the production of high quality research results and highly skilled researchers at PhD and Post doc level.

The research carried out in CERE is funded by grants from a number of public and private sponsors. The external funding received in 2014 fell under the following projects and categories (all amounts in kEUR):



## Total external funding

# 5074



# Conference Contributions & Invited Speakers

## JANUARY

*UTCCS-2 Meeting, Austin, Texas, USA, 28-29 January, 2014*

Jozsef Gaspar, Kaj Thomsen, Nicolas von Solms, Philip Loldrup Fosbøl, “Cape-open standard for plant wide carbon capture simulation”, UTCCS-2 Meeting, Austin, Texas, USA, 28-29 January, 2014 (oral)

## FEBRUARY

*12th International Bologna Conference on Magnetic Resonance in Porous Media, Wellington, New Zealand. 9-13 February 2014*

K. Katika, M. Adassi, M.M. Alam, I.L. Fabricius, “Differences in the Texture of Chalk as observed by NMR” 12th International Bologna Conference on Magnetic Resonance in Porous Media, Wellington, New Zealand. 9-13 February 2014 (poster)

## MARCH

## APRIL

*Fourth EAGE Shale Workshop, Porto, Portugal, 6-9 April, 2014*

E.N. Mbia, I.L. Fabricius, F. Frykman, A. Krogsbøll, and F. Dalhoff, “Quantifying Porosity, Compressibility and Permeability in Shale”, Fourth EAGE Shale Workshop, Porto, Portugal, 6-9 April, 2014 (oral)

*GeNeDis – 1st World Congress on Geriatrics and Neurodegenerative Diseases Research, Corfu, Greece, 10-13 April, 2014*

Georgios M. Kontogeorgis, “The role of Chemical Engineering in Medicinal Research including Alzheimer’s”, GeNeDis – 1st World Congress on Geriatrics and Neurodegenerative Diseases Research, Corfu, Greece, 10-13 April, 2014 (oral)

*SPE Improved Oil Recovery Symposium, Tulsa, Oklahoma, USA, 12-16 April 2014*

Wei Yan, Michael L. Michelsen, Erling H. Stenby, ”Negative Flash for Calculating the Intersecting Key Tie-lines in Multicomponent Gas Injection”, SPE Improved Oil Recovery Symposium, 12-16 April 2014, Tulsa Oklahoma, USA (oral)

*SAFT Meeting 2014. From SAFT to Experiment and Back”, Troia, Portugal, 22-24 April, 2014*

Georgios M. Kontogeorgis, “Limitations and Challenges of the SAFT approach from the practical point of view”, SAFT Meeting 2014. From SAFT to Experiment and Back”, Troia, Portugal, 22-24 April, 2014 (oral)

Thanh-Binh Nguyen, Jean-Charles de Hemptinne, Benoit Creton, Georgios M. Kontogeorgis, “An improved GC-PPC-SAFT for LLE of hydrocarbons and oxygenated compounds in water with applications to Kow”, SAFT Meeting 2014. From SAFT to Experiment and Back”, Troia, Portugal, 22-24 April, 2014 (oral)

Xiaodong Liang, Wei Yan, Kaj Thomsen, and Georgios M. Kontogeorgis, “PC-SAFT in modeling speed of sound”, SAFT Meeting 2014. From SAFT to Experiment and Back”, Troia, Portugal, 22-24 April, 2014 (oral)

Xiaodong Liang, Ioannis Tsivintzelis, and Georgios M. Kontogeorgis, “Modeling water containing systems with the simplified PC-SAFT and CPA EOS”, SAFT Meeting 2014. From SAFT to Experiment and Back”, Troia, Portugal, 22-24 April, 2014 (poster)

Martin G. Bjørner; Gürkan Sin; Georgios M. Kontogeorgis; “Uncertainty analysis and derivative properties in advanced equations of state”, SAFT Meeting 2014. From SAFT to Experiment and Back”, Troia, Portugal, 22-24 April, 2014 (oral)

Martin G. Bjørner; Gürkan Sin; Georgios M. Kontogeorgis; “Uncertainty analysis and derivative properties in advanced equations of state”, SAFT Meeting 2014. From SAFT to Experiment and Back”, Troia, Portugal, 22-24 April, 2014 (poster)

## MAY

*Interpore 27-30 May, 2014, Milwaukee, USA*

E. Rosenbrand, I.L. Fabricius, “Quantification of sandstone pore geometry by means of image analysis: applications for geothermal energy storage”, Interpore 27-30 May, 2014, Milwaukee, USA (oral)

## JUNE

*ARMA 14-7169 American Rock Mechanics Association The 48th US Rock Mechanics / Geomechanics Symposium, Minneapolis, MN, USA, 1-4 June 2014*

J.B. Regel, I. Orozova-Bekkevold, I.L. Fabricius, “Effective Stresses in the Hejre Field, North Sea”, ARMA 14-7169 American Rock Mechanics Association The 48th US Rock Mechanics / Geomechanics Symposium, Minneapolis, MN, USA, 1-4 June 2014 (oral) K.A. Andreassen, “Strength and Biot’s Coefficient for High-Porosity Oil- or Water-Saturated Chalk”, ARMA 14-7169 American Rock Mechanics Association The 48th US Rock Mechanics / Geomechanics Symposium, Minneapolis, MN, USA, 1-4 June 2014 (poster)

*21st World Petroleum Congress, Moscow, Russia, 15-19 June, 2014*

Ioannis Xiarchos, Philip Loldrup Fosbøl , Mohammad Monzurul Alam, Lykourgos Sigalas, Chaudhary Bilal Shaukat, Ida Lykke Fabricius, Alexander Shapiro, Kaj Thomsen, “Smart Water Flooding Experiments with Automated Equipment for Inline Resistivity and Sound Velocity Measurements”, 21st World Petroleum Congress, 15-19 June 2014, Moscow, Russia (Poster & 15 min presentation)

*76th EAGE Conference & Exhibition 2014. Amsterdam RAI, The Netherlands, 16-19 June 2014*

M.M. Alam, K. Katika, I.L. Fabricius, ”Effect of salinity and specific ions on amount of bound water on quartz, calcite and kaolinite, as observed by NMR transverse relaxation time (T2)”, 76th EAGE Conference & Exhibition 2014, Amsterdam RAI, The Netherlands, 16-19 June 2014 (oral)

A. Awadalkarim, N.N. Foged, I.L. Fabricius, “Elastic deformation behaviour of Palaeogene clay from Fehmarn Belt area”, 76th EAGE Conference & Exhibition 2014 Amsterdam RAI, The Netherlands, 16-19 June 2014 (oral)

## JULY

*27th European Symposium on Applied Thermodynamics (ESAT), Eindhoven, The Netherlands, 6-9 July, 2014*

Martin G. Bjørner, Georgios M. Kontogeorgis, “Utilization of derivative properties for the estimation of pure compound parameters of CO<sub>2</sub> with the CPA EoS and a quadrupole CPA EoS”, 27th European Symposium on Applied Thermodynamics (ESAT), Eindhoven, The Netherlands, 6-9 July, 2014 (oral) Fragkiskos Tzirakis, Georgios Kontogeorgis, Nicolas von Solms, Christophe Coquelet, Paolo Stringari, “Experimental data for CO<sub>2</sub> + N<sub>2</sub> + TBAB + H<sub>2</sub>O hydrate system”, 27th European Symposium on Applied Thermodynamics (ESAT), Eindhoven, The Netherlands, 6-9 July 2014 (oral)

Igor Nesterov, Alexander Shapiro, Georgios Kontogeorgis, “Development of multicomponent potential adsorption theory in application to binary mixtures containing polar compounds”, 27th European Symposium on Applied Thermodynamics (ESAT), Eindhoven, The Netherlands, 6-9 July 2014 (oral) Susana Almeida, Luis González Martos, Jordi Brull Costa, Rasmus Lundsgaard, Georgios Kontogeorgis, Jacob Sonne, Christian Wang,

Adam Rubim, Nicolas von Solms, “Predictive Modeling of Gas Diffusion and Solubility in Polymers for Offshore Application”, 27th European Symposium on Applied Thermodynamics (ESAT), Eindhoven, The Netherlands, 6-9 July, 2014 (poster)

*International Symposium on Solubility Phenomena and Related Equilibrium Processes (ISSP 16), Karlsruhe, Germany, 21-25 July, 2014*

Kaj Thomsen, Muhammad Waseem Arshad, ”Thermodynamic modeling of CO<sub>2</sub> capture system with liquid-liquid phase split in addition to VLE and SLE”, International Symposium on Solubility Phenomena and Related Equilibrium Processes (ISSP 16), 21-25 July, 2014, Karlsruhe, Germany (oral) ICCT SAICHe Conference 2014, 27 July - 1 August, 2014, Durban, South Africa

Georgios M. Kontogeorgis, “Equations of State in Three Centuries - What have we learnt ? What more needs to be done?”, ICCT SAICHe Conference 2014, 27 July - 1 August, 2014, Durban, South Africa

Peter Jørgensen Herslund, Kaj Thomsen, Jens Abildskov, Nicolas von Solms, Aurélie Galfré, Pedro Brântuas, Matthias Kwaterski and Jean-Michel Herri, “Modelling and Measuring Hydrate Promotion for CO<sub>2</sub> Capture,” ICCT SAICHe Conference 2014, 27 July - 1 August, 2014, Durban, South Africa

Susana Almeida, Jordi Brull Costa, Luis Gonzalez, Rasmus Lundgaard, Georgios Kontogeorgis, Adam Rubin, Christian Wang, Jacob Sonne, Nicolas von Solms, “Gas Permeability and Solubility in Polymers for Offshore Pipelines,” ICCT SAICHe Conference 2014, 27 July - 1 August, 2014, Durban, South Africa

*ICGH8 - International Conference on Gas Hydrates (ICGH8-2014),Beijing, China, 28 July - 1 August, 2014*

Christine Malmos Perfeldt, Pei Cheng Chua, Nagu Daraboina, Dennis Friis, Erlend Kristiansen, Hans Ramløv, John M. Woodley, Malcolm A. Kelland, and Nicolas von Solms, “Inhibition of Gas Hydrate Formation with a Hyperactive Insect Antifreeze Protein”, International Conference on Gas Hydrates (ICGH8-2014),Beijing, China, 28 July - 1 August, 2014 (poster)

Peter Jørgensen Herslund, Kaj Thomsen, Jens Abildskov, Nicolas von Solms, Aurélie Galfré, Pedro Brântuas, Matthias Kwaterski and Jean-Michel Herri, “Modelling and Measuring Hydrate Promotion for CO<sub>2</sub> Capture,” International Conference on Gas Hydrates (ICGH8-2014),Beijing, China, 28 July - 1 August, 2014 (poster)

Nagu Daraboina, Peter Jørgensen Herslund, Nicolas von Solms, “The combined effect of thermodynamic promoters THF and cyclopentane on the kinetics of flue gas hydrate formation,” International Conference on Gas Hydrates (ICGH8-2014),Beijing, China, 28 July - 1 August, 2014 (poster)

Galfre Aurélie, Brantuas, Pedro, Cameirao Ana, Ouabbas Yamina, Herri Jean-Michel, Herslund Peter, von Solms Nicolas, “CO<sub>2</sub> capture by using hydrates: 1) the benefice and the counterpart of thermodynamic additives,” International Conference on Gas Hydrates (ICGH8-2014),Beijing, China, 28 July - 1 August, 2014 (poster)

Nagu Daraboina; Nicolas von Solms, “Experimental Evaluation of Kinetic Inhibitors for Natural Gas Hydrate Formation in the presence of n- heptane,” International Conference on Gas Hydrates (ICGH8-2014),Beijing, China, 28 July - 1 August, 2014 (poster)

Fragkiskos Tzirakis, Nicolas von Solms, Georgios Kontogeorgis, Christophe Coquelet, Paolo Stringari, “Experimental Data For CO<sub>2</sub> Hydrate Promotion,” International Conference on Gas Hydrates (ICGH8-2014),Beijing, China, 28 July - 1 August, 2014 (poster)



# Conference Contributions & Invited Speakers

Nagu Daraboina, Praveen Linga, John Ripmeester, Virginia K Walker, Peter Englezos, “The Unusual Growth Behavior of Methane/Ethane/Propane Hydrate Crystals in the Presence of Inhibitor at low pressure,” International Conference on Gas Hydrates (ICGH8-2014),Beijing, China, 28 July - 1 August, 2014 (poster)

AUGUST

21st International Congress of Chemical and Process Engineering CHISA 2014 Prague - 17th Conference on Process Integration, Modelling and Optimisation for Energy Saving and Pollution Reduction PRES 2014, 23-27 August 2014 Prague, Czech Republic

Georgios M. Kontogeorgis, “One century with association models – what have we learnt”, 21st International Congress of Chemical and Process Engineering CHISA 2014 Prague - 17th Conference on Process Integration, Modelling and Optimisation for Energy Saving and Pollution Reduction PRES 2014, Prague, Czech Republic, 23-27 August 2014 (oral)

ECTP2014, 20th European Conference on Thermophysical Properties, 31 August - 4 September 2014, Porto, Portugal

T. Regueira, V. Vs, A.S.B. Morcous, E.H. Stenby, W. Yan, „Density and viscosity measurement for systems related to high pressure high temperature reservoirs”, ECTP2014, 20th European Conference on Thermophysical Properties, 31 August - 4 September 2014, Porto (Portugal) (poster)

SEPTEMBER

ECMOR IV, 14th European Conference on the Mathematics of Oil Recovery, Catania, Sicily, Italy 8-11 September 2014

S.M. Nielsen, I. Nesterov, A. A. Shapiro, “Microbial Enhanced Oil Recovery – A Mathematical Study of the Potential of Spore-forming Bacteria”, ECMOR IV, 14th European Conference on the Mathematics of Oil Recovery, Catania, Sicily, Italy 8-11 September 2014 (oral)

92nd Annual Meeting Deutsche Mineralogische Gesellschaft (DMG) 2014, 21-24 September 2014, Jena, Germany

E. Rosenbrand, S. Sindern, I.L. Fabricius, L. Gronen, F.M. Meyer, “Automated quantitative mineralogy of sandstones – examples of QEMSCAN applications for the study of hot water storage in geothermal aquifers and diagenesis.” DMG 2014 Abstract, 92nd Annual Meeting Deutsche Mineralogische Gesellschaft (DMG) 2014, from 21-24 September 2014 in Jena, Germany (oral)

OCTOBER

International Conference on Greenhouse Gas Technologies, GHGT 12, Austin, TX, USA, 5-9 October, 2014

Jozsef Gaspar, Kaj Thomsen, Nicolas von Solms, Philip Loldrup Fosbøl, “Solid formation in piperazine rate-based simulation”, International Conference on Greenhouse Gas Technologies, GHGT 12, Austin, TX, USA, 5-9 October, 2014 (oral)

Jozsef Gaspar, Muhammad Waseem Arshad, Eirik Ask Blaker, Birger Langseth, Tord Hansen, Kaj Thomsen, Nicolas von Solms, Philip Loldrup Fosbøl, “A low energy aqueous ammonia CO<sub>2</sub> capture process”, International Conference on Greenhouse Gas Technologies, GHGT 12, Austin, TX, USA, 5-9 October, 2014 (oral)

Philip Loldrup Fosbøl, Jozsef Gaspar, Sören Ehlers, Alfons Kather, Patrick Briot, Michel Nienoord, Purvil Khakharia, Yann Le Moullec, Olaf T. Berglihn, Hanne Kvamsdal, “Solid formation in piperazine rate-based

simulation”, International Conference on Greenhouse Gas Technologies, GHGT 12, Austin, TX, USA, 5-9 October, 2014 (oral)

IEEE Conference on Control Applications (CCA), 2120-2126, 2014, IEEE, 2014 IEEE Multi-Conference on Systems and Control, Antibes, France, 8-10, 2014

L.N. Petersen, N.K. Poulsen, H.H. Niemann, C. Utzen, J.B. Jørgensen, “Application of Constrained Linear MPC to a Spray Dryer”, Proceedings of the 2014 IEEE Conference on Control Applications (CCA), 2120-2126, 2014, IEEE, 2014 IEEE Multi-Conference on Systems and Control, Antibes, France, 8-10, 2014

The Ninth Annual Conference on the Physics, Chemistry and Biology of Water, 9-12 October, 2014, Pamporovo, Bulgaria

Georgios Kontogeorgis, “Thermodynamics of Water and Water Solutions – Questions, Myths and some Answers”, The Ninth Annual Conference on the Physics, Chemistry and Biology of Water, 9-12 October, 2014, Pamporovo, Bulgaria (oral)

The 35th Workshop & Symposium of IEA Collaborative Project on EOR, Beijing, China 15-17 October 2014

Wei Yan, Michael L. Michelsen, Erling H. Stenby, “Efficient Phase Equilibrium Calculation for Compositional Reservoir Simulation of Gas Injection”, The 35th Workshop & Symposium of IEA Collaborative Project on EOR, Beijing, China 15-17 October 2014 (oral)

Erling H. Stenby, Session chairman and Executive Committee meeting, The 35th Workshop & Symposium of IEA Collaborative Project on EOR, Beijing, China 15-17 October 2014 (oral)

NOVEMBER

Microbial Enhanced Oil Recovery (MEOR): From Theory to Field Implementation, Stavanger, Norway, 18 November, 2014

S.M. Nielsen, I. Nesterov, A.Y. Halim, A.E. Lantz, A.A. Shapiro, MEOR – From an Experiment to a Model. FORCE EOR Competence Group: Microbial Enhanced Oil Recovery (MEOR): From Theory to Field Implementation, Stavanger, Norway, 18 November, 2014 20th Reservoir Microbiology Forum (RMF), London, United Kingdom, 18-19 November, 2014

Amalia Halim, Sidsel Marie Nielsen, Anna Eliasson Lantz, and Alexander Shapiro, “Optimization of Spore Forming Bacteria Flooding for Enhanced Oil Recovery in North Sea Chalk Reservoir”, 20th Reservoir Microbiology Forum (RMF), London, United Kingdom, 18-19 November, 2014 (oral)

SPE/PAPG Annual Technical Conference 2014, Islamabad, Pakistan, 25-26 November, 2014

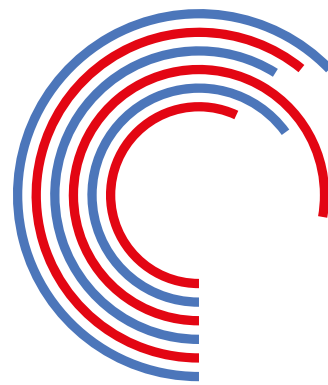
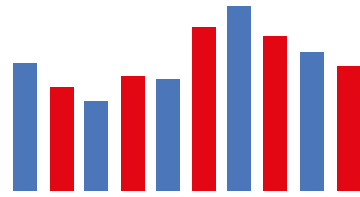
C. Bilal Shaukat, L. Sigalas, Philip Fosbøl, M. Khalid Latif, I. Xiarchos, A. Shapiro, “Effect of Salinity on Waterflooding of Petroleum Reservoirs”, SPE/PAPG Annual Technical Conference 2014, Islamabad, Pakistan, 25-26 November, 2014 (oral)

DECEMBER

53rd IEEE Conference on Decision and Control (CDC 2014), Los Angeles, USA, 15-17 December, 2014

L.N. Petersen, N.K. Poulsen, H.H. Niemann, C. Utzen, J.B. Jørgensen, “Economic Optimization of Spray Dryer Operation using Non-linear Model Predictive Control”, Proceedings of the 53rd IEEE Conference on Decision and Control, 2014, 53rd IEEE Conference on Decision and Control (CDC 2014), Los Angeles, USA, 15-17 December, 2014 (oral)





## Master Theses 2014

### Alexander Kolveit

“Investigating kinetic hydrate inhibition with antifreeze proteins”

### Louis Wilhelm Øckenholt Larsen

“Technical and economic analysis of standardizing specifications for components in fresh water generators”

### Douglas Allan Ross Milne

“An evaluation of the potential for injecting produced water to aid the artificial lift systems in offshore heavy oil production”

### Stylianos Pachitsas

“The effect of oil on hydrate formation in natural gas pipelines”

### Christian Vilhelm Prag

“Production of natural methane hydrate by CO<sub>2</sub> hydrate swapping”

### Martin Patrick Beagan Ring

“Production of natural gas from hydrates with and without CO<sub>2</sub> capture”

### Luis Gonzalez Martos

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

### Anders Schlaikjer

“Towards a predictive CPA equation of state for chemical applications”

### Ahmed Khader Ahmed Al-Alwan

“Rate dependence of oil- and water-saturated chalk”

### Stephanie Victoria Odette Mesker

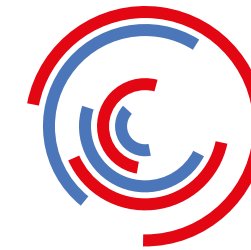
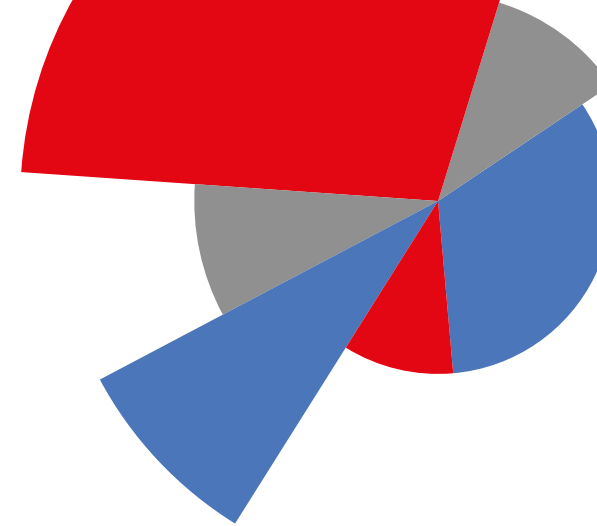
“Optimization of energy rich processes in refining using KPI´s”

### Sadek Ismail Idkedek

“Triaxial Tests at High Temperature Related to drilling engineering”

### Torsten Stilling

“BSEM and AFM of diatomite and greensand”



### David Hamrah

“Calculation of minimum miscibility pressure using fast slintube simulation”

### Karolina Kleani

“Oil Characterization by Combining Physical Distillation and Simulated Distillation”

### Dimitrios Tsolakis

“Oil Characterization by Combining Physical Distillation and Simulated Distillation”

### Varun Vs

“Study of PVT Properties of Hydrocarbon Mixtures at High Pressures”

### Amir Saad Boulos Morcous

“Study of PVT Properties of Hydrocarbon Mixtures at High Pressures”

### Abdulmecit Araz

“Experimental Study of Combined Low Salinity and Surfactant Flooding Effect on Oil Recovery”

### Martin Jørgen Einarsve

“Numerical Modelling of Oil Production by Smart Waterflooding”

### Sadek Idkedek

“Triaxial Tests at High Temperature Related to Drilling Engineering”

### Karim Almoor

“Thermodynamic modeling of CO<sub>2</sub> capture process based om amine mixture”

### Mikael Refshammer Sørensen

“Processing of rare earth element ore: Thermodynamic modeling and simulation”

### Hosein Aray

“Production optimization and simulation of oil reservoirs”

### Alexander Forsberg

“Elasticity of water-saturated sandstone at higher temperature”



Publications 2014



Previously submitted manuscripts

**SEP 0812**      *“Permeability, Diffusivity and Solubility of Carbon Dioxide in Fluoropolymers: An Experimental and Modeling Study”*

Vasu Neela, and Nicolas von Solms  
(Journal of Polymer Research, 21 (2014) 401-)

**SEP 0908**      *“Addition of Malodorants to Lighter Gas – The Phase Equilibrium properties of Mixtures og Lighter Gas and Selected Substances”*

Vasu Neela, and Nicolas von Solms  
(Chemical Engineering Research and Design, 92 (2014) 1851-1860)

**CERE 1119**      *“Crossflow and Water Banks in Viscous Dominant Regimes of Waterflooding”*

Hao Yuan, Xuan Zhang, Alexander Shapiro, and Erling Stenby (Petroleum Science and Technology, 32(10) (2014) 1227-1232)

**CERE 1311**      *“Experimental Study of Bacterial Penetration into Chalk Rock: Mechanisms and Effect on Permeability”*

Amalia Halim, Alexander Shapiro, Anna Eliasson Lantz, and Sidsel Marie Nielsen (Transport in Porous Media Journal, 101(1) (2014) 1-15)

**CERE 1322**      *“Synthesis Methods in Phase Equilibria: A New Apparatus and Error Analysis of the Method”*

José M.S. Fonseca, and Nicolas von Solms  
(Journal of Supercritical Fluids, 86 (2014) 49-56)

**CERE 1323**      *“Inhibition of Gas Hydrate Nucleation and Growth: Efficacy of an Antifreeze Protein from the Longhorn Beetle Rhagium Mordax”*

Christine Malmos Perfeldt, Pei Cheng Chua, Nagu Daraboina, Dennis Friis, Erlend Kristiansen, Hans Ramløv, John Woodley Malcolm A. Kelland, and Nicolas von Solms  
(Energy & Fuel, 28 (2014) 3666-3672)

**CERE 1327**      *”Simulations of Microbial Enhanced Oil Recovery: Adsorption and Filtration”*

Sidsel M. Nielsen, Igor Nesterov, and Alexander A. Shapiro (Transport in Porous Media, 102 (2014) 227-259)

**CERE 1333**      *“Development and Analysis of the Original UNIFAC-CI Model for Prediction of Vapor-Liquid and Solid-Liquid Equilibria”*

Azizul Azri Bin Mustaffa, Rafiqul Gani, and Georgios M. Kontogeorgis (Fluid Phase Equilibria, 366 (2014) 24-44)

**CERE 1334**      *“A Comprehensive Framework for Surfactant Selection and Design for Emulsion Based Chemical Product Design”*

Michele Mattei, Georgios M. Kontogeorgis, and Rafiqul Gani (Fluid Phase Equilibria, 362 (2014) 288-299)

**CERE 1335**      *“The Role of Monomer Fraction Data in Association Theories – can we improve the Performance for Phase Equilibria Calculations?”*

Ioannis Tsivintzelis, David Bøgh, Eirini Karakatsani, and Georgios M. Kontogeorgis (Fluid Phase Equilibria, 365 (2014) 112-122)

**CERE 1336**      *“Negative Flash for Calculating the Intersecting Key Tielines in Multicomponent Gas Injection”*

Wei Yan, Michael L. Michelsen, and Erling H. Stenby (I&EC Research, 53 (2014) 14094-14112)

**CERE 1339**      *Vapor-Liquid Equilibrium of Methane with Water and Methanol. Measurements and Modeling”*

Michael Frost, Eirini Karakatsani, Nicolas von Solms, Dominique Richon, and Georgios M. Kontogeorgis (Journal of Chemical & Engineering Data, 59 (2014) 961-967)

**CERE 1342**      *“Improving GC-PPC-SAFT Equation of State for LLE of Hydrocarbons and Oxygenated Compounds with Water”*

Thanh-Binh Nguyen, Jean-Charles de Hemptinne, Benoit Creton, and Georgios M. Kontogeorgis (Fluid Phase Equilibria, 372 (2014) 113-125)

**CERE 1343**      *“On Solving the Rachford-Rice Equation with Higher Order Methods”*

Wei Yan, and Erling H. Stenby (Fluid Phase Equilibria, 363 (2014) 290-292)

**CERE 1347**      *“Permeability, Compressibility and Porosity of Jurassic Shale from the Norwegian-Danish Basin”*

Ernest N. Mbia, Ida L. Fabricius, Anette Krogsbøll, Peter Frykman, and Finn Dalhoff (Petroleum Geoscience, 20 (2014) 257-281)

**CERE 1348**      *”Caprock Compressibility and Permeability and the Consequences for Pressure Development in CO<sub>2</sub> storage sites”*

Ernest N. Mbia, Peter Frykman, Carsten B. Nielsen, Ida L. Fabricius, Gillian E. Pickup, and Christian Bernstone (International Journal of Greenhouse Gas Control, 22 (2014) 139-153)



Publications 2014

CERE 1349	<i>“Equilibrium Total Pressure and CO<sub>2</sub> Solubility in Binary and Ternary Aqueous Solutions of 2-(Diethylamino)ethanol (DEEA) and 3-(Methylamino)propylamine (MAPA)</i>
	Muhammad Waseem Arshad, hallvard Frøsne Svendsen, Philip Loldrup Fosbøl, Nicolas von Solms, and Kaj Thomsen (Journal of Chemical & Engineering Data, 59 (2014) 764-774)

CERE 1350	<i>“Equilibrium Solubility of CO<sub>2</sub> in Alkanolamines”</i>
	Muhammad Waseem Arshad, Philip Loldrup Fosbøl, Nicolas von Solms, Hallvard Fjøsne Svendsen, and Kaj Thomsen (Energy Procedia, 51 (2014) 217-223)

New manuscripts

CERE 1401	<i>“The Virtual Product-Process Design Laboratory for Structured Chemical Product Analysis and Design”</i>
	M. Mattei, N.A. Yunus, S. Kakakul, G.M. Kontogeorgis, J.M. Woodley, K.V. Gernaey, and R. Gani (Submitted for publication)

CERE 1402	<i>“History Matching with Geostatistical Prior: A Smooth Formulation”</i>
	Y. Melnikova, K. Lange, A. Zunino, K.S. Cordua, and K. Mosegaard (Mathematics of Planet Earth, Springer Berlin Heidelberg, 703-707)

CERE 1403	<i>“Process Design of Industrial Triethylene Glycol Processes using the Cubic-Plus-Association (CPA) Equation of State”</i>
	Alay Arya, Bjørn Maribo-Mogensen, Ioannis Tsivintzelis, and Georgios M. Kontogeorgis (I&EC Research, 53(29) (2014) 11766-11778)

CERE 1404	<i>“The Role of Chemical Engineering in Medicinal Research including Alzheimer’s”</i>
	Georgios M. Kontogeorgis (P.Vlamos, A. Alexiou (eds.), GeNeDis 2014, Advances in Experimental Medicine and Biology 821, 57-62)

CERE 1405	<i>“Modeling Water Containing Systems with the Simplified PC-SAFT and CPA Equations of State”</i>
	Xiaodong Liang, Ioannis Tsivintzelis, and Georgios M. Kontogeorgis (Ind.Eng.Chem. Res., 53(37) (2014) 14493-14507)

CERE 1406	<i>“Modelling of Tetrahydrofuran Promoted Gas Hydrate Systems for Carbon Dioxide Capture Processes”</i>
	Peter Jørgensen Herslund, Kaj Thomsen, Jens Abildskov, and Nicolas von Solms (Fluid Phase Equilibria, 375 (2014) 45-65)

CERE 1407	<i>”Modelling of Cyclopentane Promoted Gas Hydrate Systems for Carbon Dioxide Capture”</i>
	Peter Jørgensen Herslund, Kaj Thomsen, Jens Abildskov, and Nicolas von Solms (Fluid Phase Equilibria, 375 (2014) 89-103)

CERE 1408	<i>“Antifreeze Activity Enhancement by Site Directed Mutagenesis on an Antifreeze Protein from the Beethe Rhagium Mordax”</i>
	Dennis Steven Friis, Erlend Kristiansen, Nicolas von Solms, and Hans Ramløv (FEBS Letters, 588 (2014) 1767-1772)

CERE 1409	<i>“Porosity and Sonic Velocity Depth Trends of Eocene Chalk in Atlantic Ocean: Influence of Effective Stress and Temperature”</i>
	Ahmed Awadalkarim, and Ida L. Fabricius (Journal of Petroleum Science and Engineering, 122 (2014) 216-229)

CERE 1410	<i>“Modeling of the Pressure Propagation due to CO<sub>2</sub> Injection and the Effect of Fault Permeability in a Case Study of the Vedsted Structure, Northern Denmark”</i>
	Ernest N. Mbia, Peter Frykman, Carsten M. Nielsen, Ida L. Fabricius, Gillian E. Pickup, and Ann T. Sørensen (International Journal of Greenhouse Gas Control, 28 (2014) 1-10)

CERE 1411	<i>“Different Effects of Temperature and Salinity on Permeability Reduction by Fines Migration in Berea Sandstone”</i>
	Esther Rosenbrand, Claus Kjøller, Jacob Fabricius Riis, Frans Kets, and Ida Lykke Fabricius (Geothermics, 53 (2015) 225-235)

CERE 1412	<i>“Petrophysical and Rock-Mechanics Effects of CO<sub>2</sub> Injection for Enhanced Oil Recovery: Experimental Study of Chalk from South Arne Field, North Sea”</i>
	M. Monzurul Alam, Morten Leth Hjuler, Helle Foged Christensen, and Ida Lykke Fabricius (Journal of Petroleum Science & Engineering, 122 (2014) 468-487)

CERE 1413	<i>“Petrophysical Analysis of Siliceous Ooze Sediments, Møre Basin, Norwegian Sea”</i>
	Ahmed Awadalkarim, Morten Kanne Sørensen, and Ida Lykke Fabricius (Petrophysics, 55(4) (2014))

CERE 1414	<i>”Petroleum Geology of the Campos and Santos Basins, Lower Cretaceous Brazilian Sector of the South Atlantic Margin”</i>
	Pilar Clemente (Internal Report)



Publications 2014

CERE 1415	<p><i>“Crystallization Kinetics within a Generic Modeling Framework”</i></p> <p>Kresten T. Meisler, Nicolas von Solms, Krist V. Gernaey, and Rafiqul Gani (Chemical Engineering Technology, 37(8) (2014) 1383-1392)</p>
CERE 1416	<p><i>“Measuring and Modelling of the Combined Thermodynamic Promoting Effect of Tetrahydrofuran and Cyclopentane on Carbon Dioxide Hydrates”</i></p> <p>Peter Jørgensen Herslund, Nagu Daraboina, Kaj Thomsen, Jens Abildskov, and Nicolas von Solms (Fluid Phase Equilibria, 381 (2014) 20-27)</p>
CERE 1417	<p><i>”Experimental Validation of Kinetic Inhibitor Strength on Natural Gas Hydrate Nucleation”</i></p> <p>Nagu Daraboina, Stylianos Pachitsas, and Nicolas von Solms (Fuel, 139 (2015) 554-560)</p>
CERE 1418	<p><i>“The Combined Effect of Thermodynamic Promoters Tetrahydrofuran and Cyclopentane on the Kinetics of Flue Gas Hydrate Formation”</i></p> <p>Nagu Daraboina, and Nicolas von Solms (In press J. Chem. Eng. Data)</p>

CERE 1419	<p><i>“Burial Stress and Elastic Strain of Carbonate Rocks”</i></p> <p>Ida Lykke Fabricius (Geophysical prospecting, 62 (2014) 1327-1336)</p>
CERE 1420	<p><i>“Determination of Matrix Pore Size Distribution in Fractured Clayey Till and Assessment of Matrix Migration of Dechlorinating Bacteria”</i></p> <p>Cong Lu, Mette M. Broholm, Ida L. Fabricius, and Poul L. Bjerg (Bioremediation Journal, 18 (2014) 295-308)</p>
CERE 1421	<p><i>“On Petroleum Fluid Characterization with the PC-SAFT Equation of State”</i></p> <p>Xiaodong Liang, Wei Yan, Kaj Thomsen, and Georgios M. Kontogeorgis (Fluid Phase Equilibria, 375 (2014) 254-268)</p>
CERE 1422	<p><i>“New Variant of the Universal Constants in the Perturbed Chain-Statistical Association Fluid Theory Equation of State”</i></p> <p>Xiaodong Liang, and Georgios M. Kontogeorgis (Accepted by I&amp;EC Research)</p>

CERE 1423	<p><i>“Modeling Phase Equilibria for Acid Gas Mixtures using the Cubic-Plus-Association Equation of State. 3. Applications Relevant to Liquid or Supercritical CO<sub>2</sub> Transport”</i></p> <p>Ioannis Tsivintzelis, Shahid Ali, and Georgios M. Kontogeorgis (Journal of Chemical &amp; Engineering Data, 59(10) 2955-2972)</p>
CERE 1424	<p><i>“Modeling Water Saturation Points in Natural Gas Streams Containing CO<sub>2</sub> and H<sub>2</sub>S – Comparisons with different Equations of State”</i></p> <p>Leticia C. dos Santos, Samir S. Abunahman, Frederico W. Tavares, Victor R. R. Ahón, and Georgios M. Kontogeorgis (Accepted for publication)</p>
CERE1425	<p><i>“Two-Phase Immiscible Flows in Porous Media: The Mesoscopic Maxwell-Stefan Approach”</i></p> <p>Alexander A. Shapiro (Accepted by Transport in Porous Media)</p>
CERE 1426	<p><i>“Modeling of Dissolution Effects on Water-flooding”</i></p> <p>Artem Alexeev, Alexander Shapiro, and Kaj Thomsen (Accepted for publication in Transport in Porous Media)</p>

CERE 1427	<p><i>“A Mean-Variance Objective for Robust Production Optimization in Uncertain Geological Scenarios”</i></p> <p>Andrea Capolei, Eka Suwartadi, Bjarne Foss, and John Bagterp Jørgensen (Journal of Petroleum Science and Engineering, 2014)</p>
CERE 1428	<p><i>“Distribution of Gas Hydrate Inhibitor Monoethylene Glycol in Condensate and Water Systems: Experimental Measurement and Thermodynamic Modeling Using the Cubic-Plus-Association Equation of State”</i></p> <p>Muhammad Riaz, Mustafe A. Yussuf, Michael Frost, Georgios M. Kontogeorgis, Erling H. Stenby, Wei Yan, and Even Solbraa (Energy Fuels, 28 (2014) 3530-3538)</p>
CERE 1429	<p><i>“An Electrolyte CPA Equation of State for Mixed Solvent Electrolytes”</i></p> <p>Bjørn Maribo-Mogensen, Kaj Thomsen, and Georgios M. Kontogeorgis (Submitted for publication)</p>
CERE 1430	<p><i>“Modeling MEA with the CPA Equation of State: A Parameter Estimation Study Adding Local Search to PSO Algorithm”</i></p> <p>Leticia Cotia dos Santos, Frederico Wanderley Tavares, Victor Rolando Ruiz Ahón, and Georgios M. Kontogeorgis (Submitted for publication)</p>



Publications 2014

CERE 1431	<p>“Thermodynamic Modeling of CO<sub>2</sub> Absorption in Aqueous N-Methyldiethanolamine using Extended UNIQUAC Model”</p> <p>Negar Sadegh, Erling H. Stenby, and Kaj Thomsen (Accepted by Fuel)</p>
CERE 1432	<p>“Testing Antifreeze Protein from the Long-horn Beetle Rhagium Mordax as Kinetic Gas Hydrate Inhibitor using a High Pressure Micro Differential Scanning Calorimeter”</p> <p>Nagu Daraboina, Christine Malmos, and Nicolas von Solms (Submitted for publication)</p>
CERE 1433	<p>“Natural Gas Hydrate Formation and Inhibition in Gas/Crude Oil/Aqueous Systems”</p> <p>Nagu Daraboina, Stylianos Pachitsas, and Nicolas von Solms (Accepted by Fuel)</p>
CERE 1434	<p>“Thermodynamics of Polymer Solutions”</p> <p>G.M. Kontogeorgis, N. von Solms (Chapter for the 4th ed. of the Handbook of Colloid and Surface Chemistry, CRC Press, Editor: K. Birdi</p>

CERE 1435	<p>“Modeling Phase Equilibria for Acid Gas Mixtures using the CPA Equation of State. Part IV. Applications to mixtures of CO<sub>2</sub> with alkanes”</p> <p>Ioannis Tsivintzelis, Shahid Ali, and Georgios M. Kontogeorgis (Submitted for publication)</p>
CERE 1436	<p>“Benchmarking and Comparing First and Second Generation Post Combustion CO<sub>2</sub> Capture Technologies”</p> <p>Philip Loldrup Fosbøl, Jozsef Gaspar, Søren Ehlers, Alfons Kather, Patrick Briot, Michiel Nienoord, Purvil Khakharia, Yann Le Moullec, Olaf T. Berglihn, and Hanne Kvamsdal (Energy Procedia, 63 (2014) 27-44)</p>
CERE 1437	<p>“A Low Energy Aqueous Ammonia CO<sub>2</sub> Capture Process”</p> <p>Jozsef Gaspar, Muhammad Waseem Arshad, Eirik Ask Blaker, Birger Langseth, Tord Hansen, Kaj Thomsen, Nicolas von Solms, and Philip Loldrup Fosbøl (Energy Procedia, 63 (2014) 614-623)</p>
CERE 1438	<p>“Solid Formation in Piperazine Rate-based Simulation”</p> <p>Jozsef Gaspar, Kaj Thomsen, Nicolas von Solms, and Philip Loldrup Fosbøl (Energy Procedia, 63 (2014) 1074-1083)</p>

CERE 1439	<p>“From Abstract to Peer-reviewed Publication: Country Matters”</p> <p>Lauge Østergaard, Philip L. Fosbøl, Robert A. Harrington, Zubin J. Eapen, Eric D. Peterson, and Emil L. Fosbøl (International Journal of Cardiology 174(3), 830-832, 2014)</p>
CERE 1440	<p>“Aqueous Ammonia CO<sub>2</sub> Capture Process – Modeling and Simulation Study”</p> <p>Muhammad Waseem Arshad, Jozsef Gaspar, Philip Fosbøl, Birger Langseth, Tord Hansen, and Eirik Ask Blaker (Internal Report)</p>
CERE 1441	<p>“Wet Gas Flow Metering”</p> <p>Martin Gamel Bjørner, and Philip Loldrup Fosbøl (Internal Report)</p>
CERE 1442	<p>“Microbial Enhanced Oil Recovery – A Mathematical Study of the Potential of Spore-forming Bacteria”</p> <p>S.M. Nielsen, I. Nesterov, A.A. Shapiro (Submitted for publication)</p>

CERE 1443	<p>“Petrobras’ Process Simulator and Cubic Plus Association (CPA) Equation of State: A Tool for Flow Assurance Projects”</p> <p>Leticia C. Santos, Samir S. Abunahman, Frederico Wanderley Tavares, Victor Ahón, and Georgios Kontogeorgis (Submitted for publication)</p>
CERE 1444	<p>“Profiling of Indigenous Microbial Community Dynamics and Metabolic Activity during Enrichment in Molasses-Supplemented Crude Oil-Brine Mixtures for Improved Understanding of Microbial Enhanced Oil Recovery”</p> <p>Amalia Yunita Halim, Dorthe Skou Pedersen, Sidsel Marie Nielsen, and Anna Eliasson Lantz (Submitted for publication)</p>
CERE 1445	<p>“Enzymatically Assisted CO<sub>2</sub> Removal from Flue-Gas”</p> <p>Maria T. Gundersen, Nicolas von Solms, and John M. Woodley (Energy Procedia, 62 (2014) 624-632)</p>



# STAFF 2014

## Faculty



Ida Lykke Fabricius



Georgios M.  
Kontogeorgis



Michael L.  
Michelsen



Alexander A.  
Shapiro



Nicolas von Solms



Philip L. Fosbøl

## Associated faculty



Erling H. Stenby



Kaj Thomsen



John Bagterp  
Jørgensen



Wei Yan



Katrine Alling  
Andreasen



Klaus Mosegaard

## Scientific Staff

Sidsel Marie Nielsen  
Igor Nesterov  
Duc Thuong Vu  
Nagu Darboina  
Ioannis Xiarchos  
Teresa Regueira Muniz  
Knud Cordua  
Andrea Zunino  
Andrea Capolei  
Xiaodong Liang  
Michael Frost  
Hani Akbari  
Dariusz Lerch  
Liang Mu  
Muhammad Waseem Arshad

## Technical and Administrative Staff

Povl Valdemar Andersen  
Anne Louise Biede  
Christian Carlsson

Thoung Dang  
Hector Ampuero Diaz  
Sinh Hy Nguyen  
John Troelsen  
Karin Petersen  
Zacarias Teclé  
Patricia Wagner  
Olga Kontogeorgis  
Ane Sogaard Avlund

## PhD Students

Michael Frost  
Christine Malmos  
Morten Kanne Sørensen  
Angeliki Xenaki  
Alsu Khusainova  
Amalia Halim  
Martin Gamel Bjørner  
Krishna Hara Chakravarty  
Artem Alexeev  
Hiep Dinh Nguyen  
Lisa Pasquinnelli

Jozsef Gaspar  
Konstantina Katika  
Carolina Figueroa  
Alay Arya  
Susana Almeida  
Arne Gladis  
Farhad Varzandeh  
Anders Schlaikjer  
Tobias Orlander  
Duncan Paterson  
Casper Schytte Hemmingsen  
Diego Rolando Sandoval Lemus  
Nathan Quadrio  
Christos Tsanas  
Fragkiskos Tzirakis

## External PhD Students

Maria Gundersen Deslauriers  
Kresten Troelstrup Meisler  
Thomas Bisgaard

## External/associated staff

Allan P. Ensig-Karup  
Max La Cour Christensen  
Jens Honore Walther

## Guests

Katrine Hedegaard  
Maria Del Pilar C. Vidal  
Javeed Awan

## Other Staff

Florin Maticu  
Randi Neerup  
Mehrdad Ahkami



