

# CERE

ANNUAL  
REPORT 2017





## **CERE Annual Report 2017**

### **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

### **Editor**

Hanne Pernille Andersen,  
Center Coordinator, CERE

### **Assistant Editors**

Patricia Wagner,  
Project Administrator, CERE  
Anne Louise Biede,  
Secretary, CERE

### **Text**

Morten Andersen,  
science reporter  
[www.manjourn.dk](http://www.manjourn.dk)

### **Layout**

We Love People

### **Photos**

– unless otherwise stated  
Christian Ove Carlsson, CERE

### **Cover photo**

The Water Bridge is created when high voltage is applied across two beakers of distilled water and can reach up to 4 cm in length. This structural behaviour of water is currently debated, but may be related to the unusual properties of liquid water.

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# Challenging Year, New Opportunities

Welcome to the 2017 CERE Annual Report. 2017 was a challenging year in the energy sector. The modest oil prices continue, putting pressure on a number of our member companies. The Danish energy landscape changed with both Maersk Oil and the oil & gas section of DONG Energy being sold to international corporations. These and other changes have affected the CERE consortium, as might have been expected. We are grateful to the CERE consortium companies (past and present) for the many years of support, inspiration and collaboration resulting in mutual benefit. We hope that the companies which chose to leave the Consortium due to the aforementioned challenges or for other reasons may consider rejoining when better times come.

At CERE we address these challenges using a multi-scale approach, both in terms of tools and applications, in areas covering all the disciplines where the center has

expertise (e.g. thermodynamics, modelling, geology and geophysics), including combining them when this is possible. We believe that new CERE faculty will contribute significantly to these future developments: Assistant Professor Thomas Guldborg Petersen (DTU Civil Engineering) and Associate Professor Allan Peter Engsig-Karup (DTU Compute), the latter returning to DTU and CERE after a year in the private sector.

## **Focus on CO<sub>2</sub>, oil, gas, and water**

In this report, you will see that we continue to focus on various dimensions of CO<sub>2</sub>: capture, transport, utilization and storage. The CO<sub>2</sub> oriented projects include the EU-funded INTERACT project on CO<sub>2</sub> capture using enzyme-based solvents in collaboration with Novozymes. Further, a recently completed project on gas hydrates use for CO<sub>2</sub> capture in collaboration with MINES ParisTech in France. Also, the recently started BioCO<sub>2</sub> project on turning

CO<sub>2</sub> from biogas upgrading plants into a high-value product together with Union Engineering and Danish Gas Technology Center. And finally, a new grant from the Danish Research Council on methane production from gas hydrates by injection of CO<sub>2</sub>.

You will also see our continuous involvement in oil & gas projects reflected. Some projects are supported by our Consortium members. Examples from the recently completed PhD projects are flash computations for compositional thermal simulation of flow in porous media, phase equilibrium modeling for shale production simulation, and modeling of HPHT reservoir fluids as well as asphaltene modeling. Other projects are carried out in close collaboration with the Danish Hydrocarbon Research and Technology Center (DHRTC) covering a wide range of applications including scales and corrosion, geology, and reservoir engineering. CERE's





collaboration with DHRTC is highlighted in this year's report and include the recent emphasis on extremely low permeable Lower Cretaceous Rock, a DHRTC focus area where CERE has recently become involved in several projects.

Another recent dimension is a project granted from the Villum Foundation in Denmark on "innovative antibiotics using resonant magnetic fields." The project belongs to the field of fundamental water studies. We believe this area can yield both scientific breakthroughs and technological innovations.

#### **Synergy with chemical/pharma consortium**

Finally, following the retirement of Professor Rafiqul Gani, I have accepted to lead, in addition to CERE, another consortium consisting mostly of chemical and bio/pharmaceutical companies with interests largely in property-based synthesis

and design (process systems engineering, PSE). Presently, this consortium is called KT-Consortium. You may read more at [kt.dtu.dk/english/research/kt-consortium](http://kt.dtu.dk/english/research/kt-consortium)

The current structure has two separate consortia (CERE and KT-Consortium) each with its own objectives, priorities and deliverables to the member companies. However, there is significant synergy which we will seek to explore and enhance further in the years to come. Thus, in 2018 the CERE Discussion Meeting and KT-Consortium Annual Meeting will be held at the same venue with about one full day of mutual program, giving the opportunity for member companies and a broader range of researchers to meet, and also for investigating synergies and opportunities for future projects and collaborations.

We look forward in 2018 to an exciting year of broad collaborations and projects

ranging from blue sky research to applied and market-oriented activities.

We hope you will find the annual report useful and we appreciate any comments and suggestions.

I also hope to see you at the annual CERE Discussion Meeting 2018 in June!

Professor Georgios Kontogeorgis,  
Chairman of CERE

Professor  
Georgios  
Kontogeorgis,  
Chairman of CERE  
[gk@kt.dtu.dk](mailto:gk@kt.dtu.dk)





# Dawn of a New Diversity

CERE is going through a transition with its traditional field, oil and gas related research, being supplemented strongly by a range of new projects in geothermal energy, biofuels, water, chemical, and pharmaceutical industry.

## The CERE Discussion Meeting

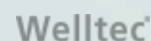
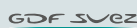
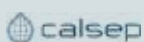
Each year, the CERE Discussion Meeting attracts a large number of both industrial and academic participants. While maintaining a strong core in thermodynamics and Enhanced Oil Recovery, the center has successfully included new fields like using drones in minerals discovery, new pathways for utilization of biogas, production of high quality CO<sub>2</sub> for industrial purposes, capture and storage of CO<sub>2</sub>, geothermal energy production and storage, and processes in the water, chemical and pharmaceutical industry sectors.

No less than 17 companies from 10 different countries were present at the 2017 version, reflecting the strength of the CERE industrial Consortium.

## The Consortium - our Strongest Asset

CERE is supported by public means from several sources, e.g. Innovation Fund Denmark, EU framework programs for science and innovation, and The Danish Research Councils. 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.







AkzoNobel Research, The Netherlands  
 BP Chemicals Limited, United Kingdom  
 Calsep, Denmark  
 Chevron, USA  
 ConocoPhillips, USA  
 Engie, France  
 ExxonMobil Research and Engineering, USA  
 Gassco AS, Norway  
 Gassnova SF, Norway  
 GDF SUEZ, France  
 Haldor Topsøe A/S, Denmark  
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Linde AG, Germany  
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 MOL, Hungary  
 National Oilwell Varco, USA  
 Petrobras S.A., Brazil  
 Schlumberger, USA  
 Shell Global Solutions International B.V.,  
 The Netherlands  
 SINOPEC, P.R. China  
 Statoil, Norway  
 Total, France  
 Union Engineering, Denmark  
 Welltec, Denmark

MOLGROUP





*From the left: Eirini Karakatsani, Thermodynamics Specialist at Topsoe; Monzurul Alam, Reservoir Geomechanics Engineer at Schlumberger; Jacob Sonne, Principal Engineer at NOV Flexibles; Miranda Mooijer, Principal Technical Expert at Shell*



### **Topsoe: A priority to be here**

As always, the CERE Discussion Meeting attracts a large number of both industrial and academic participants.

“We are a long-standing member of the CERE industry Consortium and see it as a priority to be present at the Discussion meeting,” says Dr. Eirini Karakatsani, Thermodynamics Specialist at Topsoe. Topsoe is a world leading supplier of catalysts for the chemical, energy and other industry sectors. The company’s research & development work with new and sustainable solutions for a future less dependent on fossil fuels is at a very advanced stage. Headquartered close to DTU, Topsoe tops the all-time list as workplace for the university’s candidates in chemical engineering.

The company has developed its own software for thermodynamic modelling, while also using several commercial products.

“We are dealing with a range of problems related to phase equilibria of both classical and more “modern” mixtures,” Eirini Karakatsani explains.

She has history with CERE from a previous Postdoc position, and as a participant in summer courses on advanced thermodynamic modelling.

“Actually, I maintain hopes of cooperation with CERE researchers on future projects. Unfortunately, thermodynamics in itself does not seem to be regarded as a “hot” topic by funding agencies, so we need to find the right angle for a joint application, possibly with other European partners.”

While she cannot disclose the specific content of such possible future projects,

Eirini Karakatsani is able to outline a number of general challenges:

“The problem of consistent phase equilibrium and chemical equilibrium calculation remains relevant to us, as does the challenge of efficient separations. The same is true for modelling of systems with electrolytes and biomolecules – here methods for estimating pure components’ properties are sometimes scarce, and their reliability is sometimes unknown. Similarly, we sometimes face a lack of reliable data on solubilities of gases.”

### **Schlumberger:**

#### **We always scout for talent**

With approx. 130,000 employees, Schlumberger is the world’s largest service provider for the energy sector. Monzurul Alam works out of London in the company’s Geomechanics Center of Excellence. The geomechanics group in Gatwick is part of Schlumberger headquarter operation and supports all operational areas around the world.

“The geo-mechanical behavior of an oil and gas reservoir and the surrounding formations can be assessed by a 3D Mechanical Earth Model. The model can provide insights which may reduce uncertainty and allow improved planning of drillings, completion and production,” says Monzurul Alam.

A 3D Mechanical Earth Model is built in PETREL™. Stress magnitude orientation, strain, and displacement in a 3D Mechanical is solved using the VISAGE™ finite element simulator, which can be directly coupled to reservoir simulators such as ECLIPSE™ and INTERSECT™.

“The 3D Mechanical Earth Model is the backbone for all geo-mechanical analyses,”





Monzurul Alam states. “We consider the other Schlumberger divisions as internal customers, and also have direct end-user clients outside the company. Input from universities, not least from CERE, is important for us when we consider development of potential future software products.”

Monzurul Alam is far from being new to the Discussion meeting as he wrote his Ph.D. in CERE.

“I witnessed the transition from the previous center into CERE. I think this was a very fortunate event. Previously, the group at DTU was strong on modelling of fluids, but fluids is only one side of oil and gas exploration. By including other side, which is the rock, you put yourself in a much better position.”

The same goes for the Discussion meeting, he notes:

“I like this years’ format, where all sessions are plenary. Previous years saw a number of parallel sessions, but I feel it is important that we in the geo-mechanical field get insights into what the researchers in fluids are doing, and vice versa.”

Last, but not least is the recruitment side of the conference.

“It is always interesting for us to scout for new talent. For instance, I myself was recruited by Schlumberger based on my work in CERE, and I don’t expect I will be the last to take that route!”

#### **NOV Flexibles: Joint experiments**

NOV Flexibles specializes in flexible pipelines. For instance, the company is one of very few suppliers worldwide capable of manufacturing flexible pipelines for deep sea oil and gas exploration.



“We see a growing demand for flexible pipelines capable of operating at high CO<sub>2</sub> pressures. This demand is driven partly by high pressure reservoirs with a high CO<sub>2</sub> content and partly by a growing interest in injection of CO<sub>2</sub>-rich fluids into reservoirs. This has spurred a current cooperation with CERE researchers,” explains Dr. Jacob Sonne, NOV Flexibles.

Permeation of CO<sub>2</sub> from inside the pipeline into the surrounding polymer layers – which give the pipeline its flexibility – cannot be avoided. This permeation is taken into account when selecting steel grades for a specific pipe to ensure safe operation through the entire pipeline lifetime.

Currently, exploration off the Brazilian and Western African coasts go as deep as 2.5 km below the ocean surface. As could be expected, the high pressures involved at such depths challenge pipeline suppliers. When NOV Flexibles began measuring the permeability at high pressures, the results confirmed their suspicions.

“We have seen in the experiments that the measured permeation rate in a pipe containing CO<sub>2</sub> at 320 bar at 94 °C does not fully match the calculated value when the permeabilities are assumed independent of pressure. Further, the measured permeabilities do not lie on a straight line in an Arrhenius plot as is often assumed,” says Jacob Sonne.

Following the joint experiments, NOV has revised its models for permeability. The resulting permeabilities agree with the measured values. Cooperation continues.

“We always need to document the permeability properties of our pipes as they are typically designed for 20-30 years

without any maintenance. If we don’t provide this documentation we don’t have any customers. But there is also a more positive angle to the tests we are doing in cooperation with CERE. A deep understanding of the mechanisms involved will hopefully allow us to design better and cheaper pipelines, thereby obtaining a competitive advantage,” says Jacob Sonne.

He attends his second CERE Discussion Meeting.

“The first time was a few years back. It is a nice opportunity for stepping back a bit from the daily tasks and have a chat with scientists and people from other companies. I get pointers to various trends. Although some presentations are quite far from my own field of work, I find it interesting to hear what others are doing. Still, I think some of the presenters could be clearer in explaining the relevance of their projects. I could probably have done a better job myself in my own presentation. We love to demonstrate our clever equations but tend to forget that’s not what most people want to hear!”





### Shell: Trace components come in focus

Miranda Mooijer is Principal Technical Expert and heads the Process Simulation Thermodynamics team at Shell.

“I was here 15 years ago, when I had just been employed at Shell. I am pleased to see that the atmosphere is just as nice. That hasn’t changed, even though the subjects of the conference are obviously very different.”

In her presentation, Miranda Mooijer challenges the CERE researchers and other Discussion meeting participants by presenting problems related to modelling of trace component behavior. As trace components, by definition, occur in low quantities in industrial contexts their behavior is difficult to grasp both experimentally and by modelling.

“Trace components are subject of increasing industrial interest. While they may not seem to impact the behavior of our main products too much, their economic importance can actually be significant,” says Miranda Mooijer, giving mercury as an example. A tiny amount of mercury may contaminate a bulk carrier which then cannot be labelled “mercury free” anymore. This induces economic losses for which the ship owner may hold the energy corporation responsible.

“Several applications of thermodynamic models such as CPA and PC-SAFT touch on multi-phase distribution in a way that is actually applicable to trace component behavior. But I often have the feeling that researchers actually have done the modeling and experiments we need, but we just don’t know how to access their results,” says Miranda Mooijer, while admitting that closing this gap is not solely the responsibility of academia:



“Some of the problems relate to how we communicate in industry. We often need to present our management and colleagues with “flashy” presentations that do not allow for too many details. For instance, it is quite common that one type of modelling will give the kind of results you hope for, while another type of modelling will show a less optimistic picture. Ideally, I would like to present a balanced picture, but this is difficult when the two types of modelling are done in completely different settings and illustrated very differently. In the world of today it is often not possible to present a multitude of pictures and tables that are not directly comparable. So, it would be helpful if researchers could develop more coherent ways of presenting their work.”

At the same time, Miranda Mooijer stresses that the research of CERE is more important than ever:

“I am pleased to see how much progress has been made since I was here 15 years ago. Thermodynamic simulations become ever more important to industry. We see a constant pressure for our production facilities to move closer to the technical boundaries in order to optimize outputs and stay competitive. This demand can only be met by the help of accurate thermodynamic models.”

### Industry input to be included in future projects

CERE chairman Georgios Kontogeorgis appreciates the industry comments during the Discussion meeting:

“We are currently very active in documenting both our experimental and software tools, and presenting these for the Consortium. For instance, we have just updated our software site. We are happy to hear that this work is in high demand from the industry members.”





The Discussion meeting included an after-dinner talk and an extensive poster session with contributions from a large number of CERE researchers.

“Both events were very well received as I saw it,” Georgios Kontogeorgis concludes.

“We got excellent input from the industry representatives. Many of these ideas will be included in future initiatives e.g. workshops on industrial problems as well as synergistic activities with other established industrial consortia such as the so-called KT-consortium at DTU Department of Chemical and Biochemical Engineering.”

#### **New frontiers opening**

Hunting for minerals with Unmanned Aerial Vehicles, or drones, is an entirely new activity for CERE. This prompts the projects’ coordinator, Senior Researcher Arne Døssing, to introduce himself as “a black sheep in CERE”.

Besides raising smiles from the audience, the expression has some truth in it, as for several years the bulk of research in the center has evolved around oil and gas. However, the CERE Discussion meeting 2017 shows that Arne Døssing’s drone project is by no means the only new frontier opening.

“The large oil-related CERE projects funded by Danish companies and Danish foundations have run out or are about to be completed. We will continue to be involved in a number of oil and gas related projects through our close cooperation with the Danish Hydrocarbon Research & Technology Center, but as the Discussion meeting clearly demonstrates, we have successfully managed to create a more diverse and flexible profile for CERE,” says Professor Georgios Kontogeorgis, Chairman of CERE.

“The core of CERE faculty involved remains the same, and while classic areas of research such as thermodynamics and Enhanced Oil Recovery are still highly active, a range of new projects have emerged.”

One large such project is the SYNFERON project focused on new pathways for utilization of biogas. Other projects target production of high quality CO<sub>2</sub> for industrial purposes, capture and storage of CO<sub>2</sub>, geothermal energy production and storage, and processes in the water, chemical and pharmaceutical industry sectors.





# New Front opens in Carbon Capture

Enzymes are able to double the efficiency of the amine MDEA, one of the candidates for large scale carbon capture.



Photo taken by Thorkild Christensen for DTU Chemical Engineering

*“It is not every day that you see projects by undergraduate students result in scientific publications. This has been the case here, partly due to the strong dedication of the students and staff.”*

Nicolas von Solms, Associate Professor, CERE

The enzyme carbonic anhydrase is able to boost the ability of N-methyl-diethanolamine (MDEA) to capture carbon dioxide from flue gases. The finding suddenly makes this amine a strong candidate for capture of carbon from thermal power plants and heavy industry, which globally is much needed in order to limit climate change. In recent years, another amine monoethanolamine (MEA) has become the number one candidate for large scale carbon capture.

“MEA is still the top candidate, but in combination with carbonic anhydrase, MDEA is back in the race,” says Associate Professor Nicolas von Solms, CERE.

In relation to carbon capture, the most interesting figure is how much CO<sub>2</sub> can be captured based on an investment of a given size. The results show carbonic anhydrase able to double this key figure for MDEA. Still, this “only” takes MDEA to 80 % of the efficiency of MEA relative to investment, but the story doesn’t end here, explains Nicolas von Solms:

“Firstly, we might be able to optimize the efficiency of the enzyme-MDEA system even further. Secondly, capture is really just half the job. In the following steps – known as stripping - the absorbent needs to release the carbon dioxide. The CO<sub>2</sub> is then stored or utilized, while the absorbent is regenerated for further capture. In other words, you cannot pick an absorbent solely based on its ability to capture a large quantity of CO<sub>2</sub> quickly. This is an important feature, surely, but you need to consider the entire capture-strip-regeneration flow.”

## One of the fastest enzymes known

In recent years, the stripping phase in carbon capture has become increasingly in focus. It has been realized that the high energy demand for the solvent regeneration is a barrier for large-scale adaptation of carbon capture. Typically, the MEA solvent with captured CO<sub>2</sub> is heated to 120 °C. MDEA is attractive, since it only requires moderate heating for desorption. The



drawback is the relatively slow capture velocity for MDEA; but this is exactly the feature improved by adding carbonic anhydrase.

“A lot of work is still needed in order to find the best overall solution. The new finding improves the case for MDEA, but it could well be that MEA or even a third absorbent finally emerges as the preferable solution,” comments Nicolas von Solms.

As the name suggests, carbonic anhydrase is dedicated to handling carbon in natural processes. For instance, during human respiration CO<sub>2</sub> is produced. This CO<sub>2</sub> needs to be released quickly from the body.

“Carbonic anhydrase is one of the fastest enzymes known. This is a highly attractive feature in relation to carbon capture, as we typically need to capture CO<sub>2</sub> from huge amounts of flue gas. Further, this enzyme is able to catalyze both the capture and the stripping.”

#### Several absorbents were considered

While carbonic anhydrase was an obvious focus from day one, the combination with MDEA was by no means given, Nicolas von Solms stresses:

“The main idea was really to see, if the enzyme could catalyze carbon capture. We were open to various absorbents. As MEA was already recognized as the strongest candidate, it would have been great if we could have improved its efficiency further. However, results were not good – we didn’t see any improvement. Some other absorbents were also considered, but we soon decided to focus on MDEA, as the improvement was really significant.”

Further, the amount of carbonic anhydrase needed to boost MDEA is modest: 1%. And the enzyme is not lost, but will be regenerated during the stripping process.

#### Important contribution from Novozymes

The study was made possible by the participation of Novozymes, world-leading manufacturer of industrial enzymes. Novozymes USA supplied the carbonic anhydrase.

“Only through Novozymes’ participation would we be able to do experiments of the scale we have. Normally, in such experiments only a few milligrams of enzyme are available for use due to the high purchase cost, but in this case Novozymes provided us with several kilograms. This obviously made a huge difference,” says Nicolas von Solms.

“As a chemical engineer the project was really interesting, since we did not just test at a tiny scale. We already had a pilot scale carbon capture facility at the DTU Chemical Engineering facility, and with some modifications we could do our campaigns there. Further, we were able to benefit from extensive work on modelling and simulation of capture processes, carried out in CERE during several earlier projects.”

#### Strong dedication from students

Besides the valuable scientific results, this and other CERE projects within carbon capture have yielded a range of excellent Master and Bachelor projects.

“It is not every day that you see projects by students result in scientific publications. This has been the case here, partly due to the strong dedication of the students and staff, and partly due to the excellent facilities and software built here over more than a decade,” Nicolas von Solms notes, summing up:

“On top of that are the European collaborations, which are always inspiring. So, all in all I see myself able to tick “check” on every parameter of a successful research program.”

#### An EU funded project

The study on enzyme enhanced MDEA carbon capture was conducted by PhD Arne Gladis, supervised by Associate Professor Nicolas von Solms, both CERE. The Technical University of Dortmund, Germany, was partner in the project, which involved two groups at DTU Chemical and Biochemical Engineering, CERE and PROSYS. Professor John Woodley coordinated the activities under PROSYS. Novozymes, world-leading manufacturer of industrial enzymes, supplied the relevant enzymes. The project was funded by the EU program on carbon capture, INTERACT, and co-funded by DTU.



Nicolas von Solms,  
Associate Professor



John Woodley,  
Professor



Arne Gladis,  
PhD student  
(completed in 2017)



# CO<sub>2</sub> is better than its Reputation

A joint industry project led by CERE will turn an overlooked resource, CO<sub>2</sub> from biogas upgrading plants, into a high-value product.

“In relation to upgrading of biogas to methane, CO<sub>2</sub> is seen as a mere waste product and is just released into the atmosphere. But at the same time, we import CO<sub>2</sub> for a range of industrial purposes. This is highly illogical!”

Per G. Kristensen, Head of Business Development at the Danish Gas Technology Centre (DGC), pinpoints the idea behind the BioCO<sub>2</sub> project.

While mainly associated with climate change, CO<sub>2</sub> is actually needed for products like beer and soft drinks, and is in high demand for welding and a range of other industrial processes.

Capture of CO<sub>2</sub> from coal-fired power plants has been the subject of vast research efforts over the latest decades. But in Denmark, another source is even more readily at hand. For some years now, production of biogas from manure and other agricultural waste products has caught on. Biogas can be upgraded into methane. This upgrading both increases the energy value of the gas which is distributed in the existing natural gas grid. During upgrading, CO<sub>2</sub> is produced as a by-product. Roughly 35 % of the biogas is CO<sub>2</sub>.

“The picture is somewhat distorted by the various Danish taxing schemes on energy products, but if you look at the basic net value without taxing, the CO<sub>2</sub> represents a value at the same order as the methane produced. In other words, the owner of the biogas upgrading plant discards roughly half the value he creates into the atmosphere!”, explains Per G. Kristensen, DGC.

## High CO<sub>2</sub> purity is required

Unfortunately, it is not possible to use the CO<sub>2</sub> from biogas upgrading directly for the various industrial purposes where

CO<sub>2</sub> is in demand. If things were that simple, utilization of this CO<sub>2</sub> would already be in place.

“Each of the purposes in question have their own specifications, but generally the requirements for purity are very high. It is a key challenge in the project to meet these specifications in an economically feasible way,” says Associate Professor Philip L. Fosbøl, CERE, Principal Investigator in BioCO<sub>2</sub>.

Besides CERE and DGC, Pentair is a partner to the project. The company specializes in plants for amine-based capture of CO<sub>2</sub>.

“As Union Engineering, we were world leading in amine-based CO<sub>2</sub> capture. A few years ago, we decided to move into

*“We mainly saw our membership of the CERE Consortium as a way of getting closer to the oil and gas industry. We hadn’t thought we would get into a collaboration with such direct implication to our core business so soon.”*

Jan Flensted Poulsen, Process & Technology Development Manager, Pentair.

biogas upgrading, as it was obvious that our technology would be well suited for that purpose also,” says Jan Flensted Poulsen, Process & Technology Development Manager at Pentair.

The strong emphasis on biogas in Danish energy policy was a contributing factor. “As several plants for upgrading of biogas

were built or commissioned, it became clear that a market for our technology was about to appear. Some small units were built earlier, but we knew that our technology is not relevant for applications at the single-farm scale. The larger the plant, the more relevant are amine-based techniques. And presently, the trend is to build more centralized facilities,” Jan Flensted Poulsen elaborates.

## First plant already sold

Until Pentair acquired Union Engineering in January 2017, the two companies had been competing for decades in the market for CO<sub>2</sub> recovery plants for breweries.

“When Union Engineering moved into the biogas business with our experience from putting far more than 500 amine plants in operation worldwide, we would have been an annoying competitor to Pentair’s membrane-based technologies more suitable for smaller units. After Pentair acquired Union Engineering, the full range of biogas upgrading facilities is covered,” says Jan Flensted Poulsen.

One of the targets in BioCO<sub>2</sub> is to have a commercially relevant plant ready by the end of the project period, meaning in 2019. But sometimes market forces move faster than expected.

“We have just sold the first plant, which will be installed in Kalundborg. This plant is

obviously not based on findings in the joint project, as BioCO<sub>2</sub> has only been operational for a few months. But we expect to sell several more plants over the next few years, and I am confident that some of these will be improved by research in the project. In this regard, it is very interesting to us that BioCO<sub>2</sub> promises to optimize the energy consumption of the process.





A low energy consumption will make the plants more sustainable and also more economical. This is the key issue for all suppliers in the market right now,” informs Jan Flensted Poulsen.

#### **Denmark - a biogas hot spot**

While Denmark is a small country, this market is of interest even for a global player like Pentair, the Process & Technology Development Manager stresses:

“Denmark is a hot spot for biogas upgrading right now. Even before the acquisition of Union Engineering, Pentair was looking at Denmark, since the public investments here are significant. But obviously, there is a limit to how much the Danish market can grow. We expect the investments here to decline somewhat in a few years. But then other markets will appear. We see interest in several other European countries and in South America, in China, in USA. Hopefully, the solutions in Denmark can prove a show case for further expansion of the technology.”

Union Engineering joined the CERE industry Consortium a few years back, and Pentair sustains the membership.

“We mainly saw our membership of the Consortium as a way of getting closer to the oil and gas industry. Actually, we hadn’t thought we would get into a collaboration with such direct implication to our core business so soon. But when CERE approached us with this idea, it didn’t take much persuasion to get us onboard,” says Jan Flensted Poulsen.

“This goes to show, how opening up to new partnerships can often lead to places you hadn’t imagined in advance. This reinforces our desire to pursue strategic collaboration with research institutions.”

#### **Consumer billing is an issue**

While high-quality CO<sub>2</sub> is the main focus

of BioCO<sub>2</sub>, the upgrading of biogas into methane is also revisited.

“Developing a better way to produce CO<sub>2</sub> from the upgrading is very fine, but obviously one needs to ensure that this doesn’t harm the quality of the methane. This is one of our main roles in the project,” says Per G. Kristensen, DGC. The Danish Gas Technology Centre is owned jointly by the Danish gas distribution operators.

“Our owners have a strong interest in Danish gas supply becoming “greener”. This will provide a more sustainable use of gas in the long run. However, we need to ensure that the methane quality stays within specifications both for the sake of private consumer safety, and as a precautionary measure for avoiding danger of explosions at industrial facilities. While safety is the responsibility of our owners, we assist them in this task.”

Besides safety, there is an economic aspect, explains Per G. Kristensen:

“For various technical reasons, methane from biogas can never reach 100% the same energy content as natural gas from the North Sea. This is not a problem in itself, but we need to ensure that the consumer is charged correctly. If the energy content is, say, 90% the consumer must be charged accordingly.”

#### **Portable plant to be built at DTU**

Together, the BioCO<sub>2</sub> partners are to build a portable plant to demonstrate the technology. The plant will be constructed at the premises of DTU Chemical and Biochemical Engineering. After completion it will be installed for periods of operation at two different locations. One location is Mølleåværket, a sewage management plant operated by Lyngby-Taarbæk Forsyning, and the other is a biogas facility at Fyn operated by Nature Energy.

#### **EUDP program**

BioCO<sub>2</sub> was initiated autumn 2017 as a 3-year effort sponsored by the EUDP program under the Danish Energy Agency. Partners are CERE, Danish Gas Technology Center (DGC), and Pentair. The Danish branch of Pentair, located in Fredericia, was formerly Union Engineering.

“We want to see the technology operated both at a facility with biogas production based on sewage, and at a facility with production based on manure from farms,” says Philip L. Fosbøl, CERE.

Besides the new production of high-quality CO<sub>2</sub>, he stresses that BioCO<sub>2</sub> will contribute to fulfilment of the ambitious Danish policy on sustainable energy:

“It seems realistic that methane from upgrading of biogas can substitute 5-7 % of the current energy consumption in Denmark. If further biomass becomes available, this number could go even higher in the future. Hopefully, BioCO<sub>2</sub> will contribute to this development by making biogas upgrading more economically attractive both to farmers and to biogas plant operators.”



Philip L. Fosbøl,  
Associate Professor



# Resistant Pathogens: **Resonant Magnetic Fields to the Rescue**

International studies suggest that application of electromagnetic fields could be a way to get the better of MRSA and other harmful, multi-resistant bacteria. A new effort at CERE will contribute to this end, while also aiming to identify the mechanism behind.

Hospitals, veterinarians and farmers have been in a constant state of alert for several years, as MRSA (Methicillin Resistant *Staphylococcus Aureus*) bacteria seem to persist and even spread despite massive counter-efforts. Pathogens able to tolerate most common antibiotics are an increasing problem, challenging health systems in the entire industrialized world. This had led some groups to look for innovative ways to tackle the problem.

“Seemingly, electromagnetic fields have an effect on pathogens. The effect is only seen at very specific frequencies, which are different for various species of microorganisms. This is actually even better news, as this means that if the method works, it will be specific. We can target only the pathogen, while leaving unharmed other microbes that are beneficial,” says Senior Researcher Nikolaj Sorgenfrei Blom, DTU Chemical Engineering.

## **An out-of-the-box idea**

The new effort at DTU is strongly inspired by an Italian study by Giovanni di Bonaventura and colleagues, published in *Future Microbiology*, 2014. The study shows an effect of exposure to low-frequency magnetic fields on certain pathogens that are known to cause critical conditions in patients diagnosed with cystic fibrosis (CF). The pathogens in question are not normally dangerous to humans, as they are suppressed by other microorganisms in the body, but in the lungs of CF patients they are able to

form so-called biofilms, which serve as protection and allow their growth.

“The magnetic field doesn’t actually kill the pathogen, but it hampers its ability to form biofilm. This very much comes down to the same thing, as without protection from the biofilm, the pathogen will no longer be resistant and can be fought with a standard antibiotic,” Nikolaj Sorgenfrei Blom explains.

Other groups, mainly in USA, have demonstrated inhibition of other types of pathogens – but with high-frequency fields.

Nikolaj Sorgenfrei Blom and his colleagues at DTU will keep an open mind, and try application of both low- and high-frequency fields, and even combinations of the two, against different bacteria.

## **A fourth phase of water?**

Nikolaj Sorgenfrei Blom executes the project in collaboration with Professor Georgios Kontogeorgis, Chairman of CERE.

“CERE is not normally associated with microbiology,” Nikolaj Sorgenfrei Blom admits. “However, the cooperation makes perfect sense, when one looks deeper into to scope of the project. While finding weapons against resistant bacteria is highly important, our ambition is to move beyond this application and demonstrate not only an effect but also find the mechanism behind. According to our hypothesis, the application of magnetic fields can cause subtle modifications to water molecules in the pathogens, which in turn affects their





*“According to our hypothesis, the application of magnetic fields can cause subtle modifications to water molecules in the pathogens, which in turn affects their ability to form biofilms, or to grow.”*

Senior Researcher Nikolaj Sorgenfrei Blom

ability to form biofilms, or to grow. In other words, water is the common denominator for the interest of Georgios Kontogeorgis and myself.”

To illustrate, Nikolaj Sorgenfrei Blom applies high voltage to two neighboring cup-size open water containers. Soon, a small bridge is formed between the containers. As voltage is increased further, the bridge spans across a few centimeters without collapse.

“You might say that the system I have just created is highly artificial, as it requires several thousand volts to form the bridge. How can this be relevant to life science applications? Well, actually the situation is not that different from what takes place at the surface of a cell membrane. Obviously, the voltage involved at the cell surface is much smaller but so is the length scale. A voltage of a hundred milli-Volts across a width of a few nano-meters corresponds quite well to this experiment. The point here is that the application of voltage has clearly altered the properties of the water.”

Measured by weight, two-thirds of the human body is water, and measured by number of molecules, we consist of 99% water.

“It is a paradox that water is known to be the key molecule in all life processes, yet it remains poorly understood. It is intriguing, how often the properties of water are different from other chemical substances. Why, just to give an example, is ice lighter than liquid water? Normally, a substance is heavier in its solid phase than as a liquid.”

#### **Water as a liquid crystal**

Recently, a relatively new hypothesis of a fourth phase for water – in between solid and liquid – has caught momentum.

Seemingly under certain conditions, the molecules in liquid water will organize in a way that resembles the fixed structure of a solid, in other words the structure in ice.

The most prominent advocate for a fourth phase of water is Dr. Gerald Pollack, University of Washington. He has introduced the term exclusion-zone water, or EZ-water. It is well known that the properties of water close to a hydrophilic surface are different from average water properties. This can be attributed to the fact that solutes are excluded from this zone, which is hence termed the exclusion-zone. Gerald Pollack suggests that EZ-water can exist several hundred micrometers away from the surface, and further that energy supply from UV light and other sources can expand the exclusion zone.

“EZ-water is a strong candidate for a fourth phase of water, which can be regarded as a gel or as a liquid crystal if you like,” Nikolaj Sorgenfrei Blom comments. “It is quite possible that application of electromagnetic fields with certain frequencies may shift the balance between this type of structured water, and the normal, less structured water in the cell of the pathogen. This could be the true explanation behind the effect seen in various studies. In any case, it would obviously be highly desirable to know the mechanism. Firstly, because this would be highly helpful for further development and optimization of an entirely new way of fighting pathogens, and secondly, because this understanding could open doors to many different applications that we cannot yet imagine.”



Nikolaj Sorgenfrei Blom,  
Senior Researcher

#### **An effort across four DTU departments**

The project is made possible by a two-year grant from the Villum Foundation. Last year, the foundation launched a new program, Villum Experiment, aiming to support out-of-the-box ideas. Applications are considered with anonymity for the applicant. This in order to ensure that the original idea is favoured regardless of the applicant's CV. The project on electromagnetic fields and resistant pathogens was selected for one of 38 grants. The foundation received 350 applications.

The project is highly interdisciplinary. Professor Søren Molin and Researcher Janus Haagenzen, DTU Biosustain, have opened their lab for the microbiological experiments, and will contribute with their expertise. Further, Professor Nils Olsen and Engineer Lars W Pedersen, DTU Space, will be important partners, as they have extensive experience in accurate generation of very specific electromagnetic fields. Experiments that relate to the fundamental research on water will be carried out at DTU Chemical Engineering.



A man with short, light-colored hair and glasses, wearing a light blue button-down shirt, is smiling and speaking into a microphone. He is positioned on the left side of the frame. In the background, there is a blurred blue light source, possibly a screen or a light fixture.

*“I found the CERE Discussion Meeting to be a great venue for out-of-the-box inspiration.”*

Hans Horikx, Advisor at DHRTC.

The CERE Discussion Meeting and other outreach activities has spurred ideas for new joint projects with the young Danish Hydrocarbon Research and Technology Centre (DHRTC).

Established in 2015, the Danish Hydrocarbon Research and Technology Centre (DHRTC) is on a mission to raise the expected total rate of oil and gas production from the reservoirs in the Danish part of the North Sea.

“Experience has shown that having a relatively narrow but application oriented scope can often be beneficial to scientific and technological development. I am confident this will also be the case for joint projects with CERE. They have a range of excellent capabilities that can be developed further within our framework,” says Hans Horikx, Advisor at DHRTC.

Located at the DTU campus in Lyngby, DHRTC is a national center with academic partners across Denmark: DTU, University of Copenhagen, University of Aalborg, University of Aarhus, and the Geological Survey of Denmark and Greenland (GEUS). Each institution has its own local focal point in relation to DHRTC. Nicolas von Solms, member of the CERE faculty, represents DTU.

With a background in reservoir engineering and previous positions in Shell and Maersk Oil, Hans Horikx recently joined DHRTC. Through his years in industry he has followed the work of CERE,



# DHRTC:

## “Transparency is a strong Asset for CERE”

not least in his former capacity as chairman of the Copenhagen chapter of the Society of Petroleum Engineers (SPE).

### Inspired by geothermal science

After joining DHRTC, one of Hans Horikx' first duties was to attend the CERE Discussion Meeting.

“I knew the activities on Enhanced Oil Recovery well from SPE, but I was pleasantly surprised to see how wide the interests of CERE actually are. For instance, I didn't know that CERE had activities in using drones for magnetic surveys, and also the level of knowledge within carbon capture, hydrates and geothermal energy impressed me.”

These subjects may seem of little relevance to DHRTC, but that is not entirely true.

“Actually, a presentation by Professor Ida Fabricius from CERE on geothermal energy has spurred an interesting idea for possible application in a North Sea hydrocarbon exploration.”

To understand the idea, one has to know the overall geology of hydrocarbon exploration in the Danish North Sea. To date, most hydrocarbon developments have been in an Upper Cretaceous chalk known as the Tor formation. While DHRTC does have a range of activities aimed at improved production from Tor chalk, the main focus is to further develop both the higher layers – the so called Ekofisk formation – and carbonate layers at greater depth, known as the Lower Cretaceous layers.

“Both the layers above and below Tor are underdeveloped in a hydrocarbon context. However, they pose several challenges.

The Lower Cretaceous layers are super tight. From the work on geothermal energy by Professor Fabricius and her colleagues we know that injection of water with a temperature different from the background temperature has implications for rock strength. Also, repeated changes in temperature – several injections over a longer period of time – can have more drastic consequences,” Hans Horikx explains.

### Injections can be “a thermal hammer”

While an initial injection may lead to stiffer chalk, repeated injections may ultimately lead to a collapse of the stiffness resulting in a much weaker structure.

“This can potentially be problematic, but in an oil and gas context it could actually be desirable to deliberately weaken the structure. A controlled regime of alternating cold and hot injections might act as a thermal hammer. You would want a limited weakening – just large enough to drive out the hydrocarbon content.”

As always, there is a distance between having an interesting idea and initiating activities that aim at realization.

“It is still early days for the specific idea, but my point here is that we wouldn't have thought of this, had we not been inspired by research in another field, namely geothermal energy. I found the CERE Discussion Meeting to be a great venue for this kind of out-of-the-box inspiration. In fact, I almost felt like a boy in a toy shop!”

### Smooth and regular contact

It goes without saying that DHRTC-CERE collaboration is not just on out-of-the-box ideas.

“For instance, a lot of our interest in the Ekofisk formation require capabilities within fluid modelling, fluid-rock interactions, fluid saturation, rock mechanics, geo-mechanical modelling etc. All core capabilities in CERE. The same can be said for Enhanced Oil Recovery in general,” says Hans Horikx, stressing that this obviously doesn't imply that CERE will always be involved in these projects:

“All five academic partners to DHRTC have their individual strongholds, and the choice of which groups to involve will always be dependent on the specific project. Further, we may – and have already – involve groups at DTU which are outside CERE. Still, CERE is certainly a very natural partner to us.”

Besides the wide range of topics at CERE, Hans Horikx credits the level of both verbal and poster presentations as seen at the annual Discussion Meeting:

“It is clear that CERE gives high priority to showing what they are doing. I guess this a logical consequence of their funding structure. The CERE Consortium has member companies from all over the world, and one needs to be transparent to attract their attention. As a CERE sponsor we also benefit from this transparency – while being aware that we are just one potential sponsor, competing with other sponsors for academic partnerships. But we do have the advantage of being geographically very nearby. This allows for a smooth and regular contact which I really appreciate.”



# Let's swap: Methane for CO<sub>2</sub>

Nature has vast amounts of methane stored inside so-called gas hydrates. Humankind has too much CO<sub>2</sub>. The idea of a new project at CERE is to swap our CO<sub>2</sub> for methane. Specifically, the CO<sub>2</sub> will replace the methane securing the stability of the hydrate, while the greenhouse gas now remains trapped.



Nicolas von Solms,  
Associate Professor

"The purpose is to develop a viable and safe method to produce methane gas from naturally occurring reservoirs of gas hydrates by injecting CO<sub>2</sub> or gas mixtures containing CO<sub>2</sub>, such as power plant flue gas," explains Associate Professor Nicolas von Solms. "The project attempts to address two urgent global issues: the future supply of energy and the threat of catastrophic climate change."

A gas hydrate molecule is in effect a "cage" in which a small molecule, most commonly methane, is trapped. CO<sub>2</sub> can act as an agent, which drives the methane out. If the process is designed smartly, the CO<sub>2</sub> molecule will be caged instead.

A previous study at CERE has shown that the hydrate swapping idea can be made to work.

"Quite another issue is of course whether this can be done in a way that is practically and economically feasible. Thanks to the new research grant we will be able to investigate that," says Associate Professor Nicolas von Solms, supervising both two new PhD students to be employed soon and postdoc Liang Mu (recently completed).

The project on hydrate swapping is funded by The Danish Council for Independent Research and has a total budget of DKK 5.7 million (EUR 750.000). It is scheduled to run from 2017-2020. Industry partner is Maersk Oil, while Korea Advanced Institute for Science and Technology (KAIST) is academic partner.

# Better Prediction of Corrosion in Pipelines

The current view on corrosion in oil pipelines is overly pessimistic. A new Postdoc project will pave the way for more accurate predictions and thus more cost-effective maintenance.

While corrosion in oil pipelines can indeed be very costly, exaggeration of the problem may also impose costs by triggering maintenance that is not really needed. A new project at CERE is to provide a more accurate basis for predictions of corrosion.

"Recent research at CERE suggests that the basic understanding of certain properties, which play a key role in pipeline corrosion, is off by a factor 20. This has a fundamental impact on the prediction of corrosion. Existing corrosion models will predict a corrosion rate which is much too high," says Associate Professor Philip L. Fosbøl, CERE.

The project will be conducted by Postdoc Carolina Figueroa Murcia, CERE, as a continuation of her previous project on "Solubility measurements of corrosion products". That project was sponsored by DHRTC, and so will her coming project on "CO<sub>2</sub> impact on corrosion product (FeCO<sub>3</sub>) solubility". The new project will be supervised by Philip L. Fosbøl and co-supervised by Associate Professor Kaj Thomsen.

Corrosion of offshore downhole equipment is often sustained by CO<sub>2</sub>

reacting with steel, producing a solid corrosion product, FeCO<sub>3</sub>. This layer significantly protects the pipeline against corrosion. However, the layer may disappear under certain conditions, opening up the pipeline surface to further corrosion. Here, the solubility of FeCO<sub>3</sub> is a key property. A way to predict corrosion is to use existing solubility data for FeCO<sub>3</sub> followed by thermodynamic modelling which is capable of determining the solubility as function of temperature, pressure, and auxiliary ions. This results in an estimation factor called the "solubility index".

"Knowing how important FeCO<sub>3</sub> solubility is for the prediction of corrosion, it is a true paradox that this property has not been firmly established to date," comments Philip L. Fosbøl.

In her previous project, Carolina Figueroa Murcia showed how the most recognized authors in the literature estimate a FeCO<sub>3</sub> solubility 20 times higher than reality. Caroline Figueroa Murcia is currently on maternity leave. She will commence the Postdoc project by spring 2018, and the project will continue until early 2020.

## Several Projects on Pipeline Corrosion

Besides the Postdoc project of Carolina Figueroa Murcia, CERE is engaged in other projects on corrosion in pipelines. These are carried out in collaboration with DTU Mechanical Engineering (lead) and IFE (Norway).



Philip L. Fosbøl,  
Associate Professor



# The full Range of Petrogeology

The geological expertise of Thomas Guldberg Petersen reaches all the way from the single borehole to regional structures.

“A classic petrogeologist” is the term chosen by Thomas Guldberg Petersen to describe his professional profile. The Assistant Professor at DTU Civil Engineering is the latest addition to CERE’s faculty.

“In my previous career, I have engaged in surveys related to very local geology, in principle just a single borehole, and all the way to estimation of the oil and gas resource potential of entire countries, or even regions.”

Moreover, Thomas Guldberg Petersen has equally solid experience from both academic research and industry, making

him an ideal participant in Joint Industry Projects at CERE.

Following his Master in petrogeology from Aarhus University, Thomas Guldberg Petersen worked in consultancy with assignments for oil and gas industry clients, mainly in relation to Norwegian and Danish fields. A significant part of these assignments involved applications of image logs.

“Contemporary image logs have a resolution so high that one can almost see the geology around the borehole directly. This contributes to knowledge of the geological structure of the field,

and is also valuable to operators mainly in evaluations of borehole stability,” Thomas Guldberg Petersen explains.

He later took a PhD position at the University of Copenhagen involving field work and seismic data analysis in relation to possible future oil and gas exploration in the High North, primarily Northeast Greenland, Svalbard, and the Barents Sea. The project was sponsored by DONG Energy.

Following his PhD degree, Thomas Guldberg Petersen joined Maersk Oil to take part, among other tasks, in supplying geological input for the company’s long-term evaluations of global hydrocarbon resources.

“This was often a challenging task, as the evaluations included countries with very limited geological information available. In some countries, geological surveys are not fully developed, or data are unavailable for many reasons. So, in this context it is really a matter of making the most of whatever data you have, be it from single boreholes or regional structures, and to combine these data.”

At CERE, Thomas Guldberg Petersen will be able to provide input to a range of projects, including oil and gas related projects coordinated by the Danish Hydrocarbon Research & Technology Center (DHRTC), projects related to geothermal energy, and other projects with a geology component.



Thomas Guldberg Petersen,  
Assistant Professor





# NEWS

## from CERE

### Algorithms for Density Gradient Theory

Density gradient theory is a popular framework for interfacial tension calculations, playing an important role in processes with more than one phase involved. A new project at CERE develops efficient algorithms for solving the density gradient theory in a planar interface.

In the project, carried out by Assistant Professor Xiaodong Liang and Professor Emeritus Michael L. Michelsen, density gradient theory is extensively evaluated and applied into various systems with different thermodynamic models: PR, CPA and PC-SAFT.

Xiaodong Liang and Michael L. Michelsen propose a new predictive approach, avoiding potential numerical problems. Further, a direct minimization method is developed for more general and wider applications without loss of efficiency.

The application, analysis and evaluation of these developments against more complex systems is ongoing. A MATLAB tool is available, and more interfaces are under development.

### Lecture: The Oilfield Chemist in Action

To produce oil and gas it is not enough to drill a well at the right location. Several chemicals are necessary for flow assurance and other crucial tasks. This was the key message as Dr. Malcolm Andrew Kelland, Department of Mathematics and Natural Science, University of Stavanger, Norway, visited CERE on March 16.

"The role of the oilfield chemist is often under-evaluated, yet they do a vital job. Chemists are needed to determine the best fluids, for safe and effective drilling and cleaning of wells, for completion and stimulation operations, for production and flow assurance issues and for separation of oil, gas and water at the process facilities," Dr. Kelland said, moving on to give an overview of the types of chemicals needed for the various operations, and of the environmental issues involved.



Photo taken by Thorkild Christensen for DTU Chemical Engineering

### Classic Course on Thermodynamic Models

More than 15 years ago, Professors Michael L. Michelsen and Jørgen Møllerup organized the first "Advanced Course on Thermodynamic Models: Fundamentals & Computational Aspects". Time hasn't diminished the relevance of this PhD summer course, which was once again well attended in 2017 with 22 participants from both academia and industry in 14 countries.

When Professor Michelsen became emeritus in 2015, the course was taken over by Senior Researcher Wei Yan and Professor Georgios Kontogeorgis.

The course is targeted both at researchers who develop and implement thermodynamic models for process simulation and at those who just want to learn how to develop and write an efficient and dynamic computer code. Further, both classical chemical engineers and engineers in other disciplines like petroleum engineering and mechanical engineering may benefit.

As usual, the course was held in August, and CERE intends to keep up this tradition in 2018.



## Carbon Capture Expert on Danish TV

High global atmospheric CO<sub>2</sub> concentrations already cause floods and extreme storms and these problems are predicted to become even larger in the future. Thus, it is natural to ask whether any technological solutions are available for reducing CO<sub>2</sub> concentrations. Associate Professor Philip Fosbøl, CERE, addressed this issue in an interview with Danish national tv-station DR on March 17.

"We have two options; either to clean our atmosphere or to help the cement, steel, and power sectors reduce their emissions," said Philip Fosbøl, adding that extracting CO<sub>2</sub> from the atmosphere – known as geo-engineering – is not yet an established method. Thus, the other option – known as carbon capture – is more realistic at short term.



Image from DR2 Deadline 17 March 2017

"We will need to phase out fossil fuels completely in the long run, and we can use old gas reservoirs for storing CO<sub>2</sub>. Eventually, we will probably need both carbon capture and atmospheric cleaning to reach negative CO<sub>2</sub>-emissions," Philip Fosbøl explained.



## Geotechnics and Geology on the Move

Under the catch phrase "Transforming DTU" several new buildings are about to be added to the Lyngby campus. One of these, B129, will offer the Geotechnics and Geology group in CERE a new workspace.

"Our present facilities at DTU Civil Engineering have never been optimal, as we share our present building, B119, with colleagues who frequently test large concrete and steel constructions. Every now and then this activity will interfere with our experiments, especially when we do long-term experiments," says Assistant Professor Katrine Alling Andreassen, member of the CERE faculty.

Examples of long-term experiments are deformation of rock samples under mechanical stress, and consolidation of clay and other types of fine-grained materials.

"These experiments often require several weeks' or even months' duration. Therefore, it is not always possible to avoid interference with other activities in our present facilities. We look very much forward to moving to the new lab, dedicated to our needs," says Katrine Alling Andreassen, adding that new building is dimensioned for possible new acquisitions of lab equipment.

Over recent years, the group has been able to upgrade its equipment, i.e. within NMR (Nuclear Magnetic Resonance), BET (Brunauer-Emmett-Teller gas adsorption), and MICP equipment for pore distribution characterization. The equipment will have designated rooms in the new lab.

B129 – located next to the group's present premises in B119 – is scheduled for inauguration in March 2018.



# NEWS

## from CERE



### Lecture: Coping with Oil and Gas Uncertainty

Since 2014, the sustained low oil prices have led to a significant reduction in exploration and development and the deferment of many capital projects worldwide. Still, future oil and gas engineers were able to find encouragement as a veteran in the business, Balakrishnan Kunjan, visited DTU on September 28 as SPE Distinguished Lecturer.

"It remains my belief that reliance on oil and gas is here to stay for the next few decades, but with the energy mix changing over time. There are going to be jobs in this industry for years to come, but those aspiring for jobs have to exercise some flexibility as to how they keep themselves employed before a pickup in job demand," said Balakrishnan Kunjan.

After his degree in geophysics and an additional MBA, Balakrishnan Kunjan began his career with Esso in Malaysia in 1977, and has worked in oil industry and related consultancy since. He is presently with Cue Energy in Melbourne, Australia.

"It remains one of the most exciting, interesting, and rewarding industries to be in. Based on my own travel and work in various basins around the world I can assure you that it can be fun!"

Besides the seminar for students, Dr. Kunjan gave a seminar for current oil and gas professionals on the topic of allocation of resources for exploration based on probabilistic predictions.

### Scientific Computing Expert Returns

After a year in the private sector, Associate Professor Allan Peter Engsig-Karup is back at DTU Compute and in CERE. His field of interest is Computational Mathematics and applications of modern scientific computing paradigms in engineering.

In CERE, Allan P. Engsig-Karup has contributed strongly to two joint industry projects, one on reservoir simulation (2011-2014), and recently the OPTION project addressing optimization of oil and gas production over entire oil fields. His experience in interdisciplinary research projects, industrial collaborations and transformation of fundamental research into innovative technology is likely to become an asset for CERE in future projects also.





## Worms and Wasps in Oil Recovery

Two innovative hydrocarbon projects at CERE in 2017 were inspired by biology. Both were undertaken in collaboration with – and sponsored by – Danish Hydrocarbon Research & Technology Center (DHRTC).

It is already a standard method during recovery in carbonate reservoirs to dissolve the chalk in close vicinity to the bore-head with hydrochloric acid (HCl). In another method, known as radial jet drilling, radial jets are used to penetrate into deeper layers.

“Our idea would be to combine the use of hydrochloric acid with radial jet drilling. The key challenge would be to ensure that the acid is effective not just close to the horizontal well, but further down along the “wormhole” created by the jet. We imagine various possible ways to do this, i.e. some form of encapsulation of the acid or other delaying mechanisms,” says Associate Professor Nicolas von Solms, CERE.

In the other innovative project, a 3-phase flow and well sampler, the WASP (well analysis + sampler) is suggested for sampling of oil, gas, and water from a platform’s individual wells.

“The device is can be used at both manned and unmanned platforms, but is especially valuable for unmanned platforms. An unmanned platform can easily have ten wells, and if

the platform begins producing too much water it is currently not possible for the offshore production supervisor to see which well is responsible,” comments Associate Professor Philip L. Fosbøl, CERE.

Both projects were under the DHRTC program “radical innovation” for projects of 3-month duration, allowing for suggestions, while the actual design of devices will require further work.



## Plenary Lectures in China and Brazil

Professor Georgios Kontogeorgis and Associate Professor Nicolas von Solms both represented CERE with invited lectures in 2017.

Nicolas von Solms gave a plenary lecture at the CAS-TWAS Symposium on Green Chemistry and Technology for Sustainable Development (GCT2017), held in Beijing, China, from 2-4 September. As his subject he chose “Transition to a Fossil-free Energy Landscape – Greener

Solutions for Gas Production and Carbon Capture and Storage”.

The following month, Professor Kontogeorgis addressed the IX Brazilian Conference CBTermo 2017 in an invited lecture entitled “Equations of State in Three Centuries – Are we closer to a single model for all applications?” The conference was held in Porto Alegre, Brazil, 23-27 October.



# NEWS

## from CERE

### Deeper into the North Sea Geology

The Lower Cretaceous layers in the Danish part of the North Sea contain substantial oil and gas reserves, but have till date been underdeveloped. Three new projects in CERE, all undertaken in collaboration with and sponsored by the Danish Hydrocarbon Research and Technology Center (DHRTC) focus on these deep reservoirs.

As the Lower Cretaceous geology is dominated by low-permeable chalk, it has been proposed to produce the reservoirs by gas injection. This is the subject of the first project, to be carried out by Postdoc Duncan

Paterson with Professor Erling H. Stenby and Senior Researcher Wei Yan as supervisors. Injected gas can achieve different extents of miscibility with reservoir oil and reduce the residual oil saturation. If complete miscibility could be obtained, the injected gas would recover 100 % of the oil.

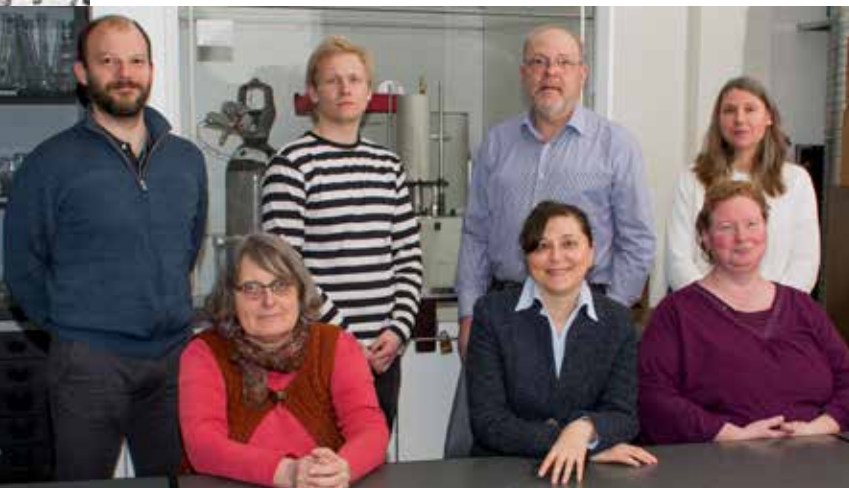
Another key topic is the influence of porous media on phase behavior. Recent field observations suggest that the saturation pressure in tight formations may change dramatically. Therefore, it is expected that the extremely low permeable Lower

Cretaceous rock may influence the phase behavior of the reservoir fluid, and this is the subject of the second project by PhD student Diego Sandaval with Senior Researcher Wei Yan and

Erling H. Stenby as supervisors. The project builds on experience from a recent shale project with ConocoPhillips.

The gas may not only be injected into the reservoir, but also liberated from the oil, as the reservoir pressure decreases. Such gas may appear in the form of bubbles, plugging the porous medium and decreasing productivity of the wells. On the other hand, the liberated gas might flow up in the reservoir and form a gas cup. This gas cup is advantageous for oil production, since it creates additional pressure. Interplay of these two alternatives (bubbles or a gas cup) may be a reason why production from the different wells at the Lower Cretaceous is so different. PhD Student Wael Almasri, under supervision of the Associate Professor Alexander Shapiro, has started a project in order to clarify what alternative actually takes place. The project is run in collaboration with GEUS, where Dr. Carsten Møller Nielsen is its co-supervisor. Close collaboration with the projects run by Wei Yan and Erling H. Stenby is planned.

Finally, a project led by Professor Ida L. Fabricius, DTU Civil Engineering, will address geology issues in relation to oil and gas exploration in the Lower Cretaceous layers in the Danish part of the North Sea.



### Former CERE Chairman to advise Total

Professor Erling H. Stenby, former Chairman of CERE, has been appointed member of the Science Council, a scientific advisory board of the energy corporation Total, headquartered in Paris, France. Total is a global integrated energy producer and provider,

a leading oil and gas company, and a major player in solar energy. The company has 98,000 employees in more than 130 countries. Total recently acquired Danish energy corporation Maersk Oil. Total is a long time member of the CERE industry Consortium.





## Welcoming the Society of Petroleum Engineers

November 21, DTU hosted a meeting of the Copenhagen section of the Society of Petroleum Engineers (SPE). The Copenhagen SPE section has representatives of all major petroleum companies operating in Denmark. It organizes six meetings per year, and according to tradition one of these is held at DTU, giving the university's researchers the opportunity to present their recent results to industry.

Senior Researcher Wei Yan of CERE, was invited to give a technical presentation on phase equilibrium in shale – a project carried out in collaboration with Conoco Philips and Exxon Mobil. Senior Researcher Hamid Nick of the Danish Hydrocarbon Research and Technology Center (DHRTC) also gave a talk on the modelling of fractures in reservoirs.

The theme of academia/industry collaboration was continued in an after-dinner talk by Associate Professor Nicolas

von Solms of CERE. He gave examples of positive experiences of long-term collaboration between CERE and its corporate partners.

This year's meeting was organized jointly by DHRTC and CERE. Further, the DTU SPE Student Chapter and its Chairman, Ph.D. Student Leonardo Meireles were active, contributing to the presence of many DTU students at the meeting. In total, around 70 participants from academia and industry were registered.

"Collaboration between the Student Chapter and the 'adult' SPE makes it possible to establish regular contacts between the students and the professionals, which is very important for the professional development of the students, and eventually, for their future employment," says Associate Professor Alexander Shapiro, CERE. Alexander Shapiro, who heads the DTU Master program in petroleum engineering, is the member of the Board of the Copenhagen Section of SPE

responsible for the organization of the SPE meetings and events at the DTU.

A relatively young tradition at the annual meetings is a poster contest organized by the SPE Student Chapter. This year's winner was Research Assistant Jyoti Pandey for his poster on the DHRTC sprint project "Radical concepts for deep reach through acid injection."

## Looking into the European Horizons

Two CERE faculty members, Associate Professors Nicolas von Solms and Philip L. Fosbøl, have been appointed reviewers for the current EU Program for Research and Innovation, Horizon 2020.

With nearly 80 billion euro of public funding, Horizon 2020 is the all-time biggest EU Research and Innovation program. The duration is 7 years – from 2014 to 2020.

## CERE to host International Oil Conference

In 2018, the annual workshop and symposium on Enhanced Oil Recovery (EOR) will be held for the 39th time by the International Energy Agency (IEA) on 3-6 September. This time this important international conference will have CERE as its host.

The topics will include studies of fluid

flow in porous media, surfactants and polymers, thermal methods, gas flooding techniques, reservoir characterization, emerging technologies, and fundamental EOR research.

Main organizer will be Professor Erling H. Stenby, member of the IEA-EOR Executive Committee, and former Chairman of CERE.





# PhD

# Defenses



# Enzymes for Carbon Capture



**Arne Berthold Gladis, PhD.**

Currently with  
Wacker Chemie, Munich

Full title:  
"Upscaling of Enzyme  
Enhanced CO<sub>2</sub> Capture"

Supervisors:  
**Nicolas von Solms,**  
**John Woodley,**  
**Philip L. Fosbøl.**

The project is a part of  
the European research  
project on carbon capture,  
INTERACT. Funding was  
provided by the European  
Commission and by DTU.

Carbon capture and storage (CCS) is the only technology that can mitigate greenhouse gas emissions from fossil fuel power. To date, high costs have been the major obstacle for industrial implementation of CCS. This project demonstrates that enzymes can enhance the ability of certain attractive solvents for carbon capture, opening up a variety of new process options for CCS.

High greenhouse gas emissions are expected in the future, as fossil fuels are the backbone of energy generation in USA, China, India and Europe, and will continue to be so for the next decades. Post-combustion carbon capture has the potential of immediately reducing emissions, as it can be retrofitted to existing plants. The captured CO<sub>2</sub> can be compressed and stored underground and is thus prevented from influencing the global temperature.

Chemical absorption is the most mature capture technology. High capital and operational costs continues to be the major

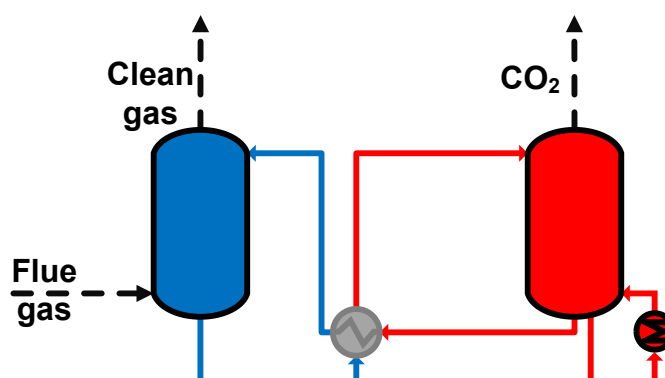
obstacle for industrial implementation. This project suggests that enzymes can be used as kinetic rate promoters that enhance the mass transfer of CO<sub>2</sub> with slow-capturing but energetically favorable solvents. Specifically, the enzyme carbonic anhydrase (CA), which enhances the mass transfer of CO<sub>2</sub> in our lungs by catalyzing the reversible hydration of CO<sub>2</sub>, is shown to be a very promising promotor for CCS. This process was previously tested successfully in lab scale and in a few cases in pilot scale, but no validated process model had been published.

The project presents the first predictive process model for enzyme enhanced CO<sub>2</sub> capture. The model accurately describes the CO<sub>2</sub> mass transfer of pilot scale experiments under a very wide range of process conditions. It showcases a successful scale-up, and the process was evaluated in both lab and pilot scale. Pilot plants experiments gave data such as temperature and solvent loading profiles as well as mass transfer rates on 71 absorption experiments with enzyme enhanced MDEA (N-methyl-diethanolamine). Further, 27 absorption experiments with the industrial standard 30 wt% MEA, as well as 37 stripgas desorption experiments, were completed.

Enzyme enhanced MDEA solutions were shown able to compete with the best solvents in terms of solvent capacity and average mass transfer. Experiments with 30 wt% MDEA carried out at 0, 0.85, and 3.5 g/L CA proved the positive effect of CA in pilot scale, where the CO<sub>2</sub> capture could be increased from 23 % to 56 %. While the enzyme enhanced MDEA did not exceed the mass transfer of the industrial standard, more than 80 % of the capture performance could be achieved with 3.5 g/L CA.

The pilot plant experiments could be accurately predicted with the in-house absorber column model CAPCO<sub>2</sub> after the kinetic enzyme model from the lab experiments was implemented. The model can very accurately simulate the influence of all parameters tested.

In conclusion, the project has clearly proven the potential of CA in CCS. The presented absorber column model can be used to simulate and optimize enzyme enhanced carbon capture and benchmark this novel technology against conventional processes.



Flow diagram for  
a solvent based  
absorption/desorption  
process for CO<sub>2</sub>  
recovery from a flue  
gas stream.



# Accurate Prediction of Asphaltene Precipitation



**Alay Arya, PhD.**

Currently postdoc and software manager at CERE and KT-Consortium, DTU

Full title:

**"Modelling of Asphaltene Systems with Association Models".**

Supervisors:

**Georgios Kontogeorgis, Nicolas von Solms.**

The project was funded by the CHIGP (Chemicals in Gas Processing) consortium (2/3) and DTU Chemical and Biochemical Engineering (1/3).

Asphaltenes are the heaviest components in reservoir oil. Much like cholesterol in human blood veins, they can cause problems if they precipitate in pipelines, production gear and at refineries. Certain conditions will promote precipitation of asphaltenes, but predictions are currently quite uncertain. The project presents several tools for improved accuracy.

Asphaltenes are characterized by high molecular weight (around 500-400 gm/mol), and they are considered the most polar components in oil. Their polar nature is imparted by the presence of heteroatoms (O, S, N, vanadium, nickel) in their structure. Asphaltenes molecules associate with each other and precipitate under certain conditions in terms of temperature, pressure and composition.

Precipitation of asphaltenes has always been a flow assurance problem to the oil industry and refineries, but in recent years the focus has become even higher, as certain Enhanced Oil Recovery (EOR) techniques involving gases may promote the precipitation. Also, more than two crudes (degassed oil) are most often mixed at the refinery inlet to either upgrade or downgrade the feedstock. This blending may cause asphaltene precipitation.

In the project, a modeling approach using the Cubic Plus Association (CPA) and Statistical Associating Fluid Theory (SAFT) equations of state (EoS's) was developed to model asphaltene precipitation. The method can predict the gas injection effect on asphaltene onset conditions. It can be used to study the EOR by gas injection prior to implementation. 3-4 experimental onset points in the relevant temperature range are required.

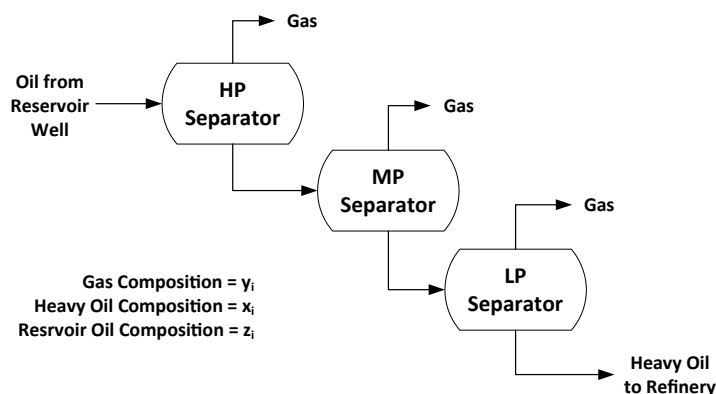
The developed approach using both CPA and PC-SAFT EoS's was compared with the literature approach based on the PC-SAFT EoS. It was found that the PC-SAFT model cannot correlate the asphaltene upper onset pressure boundary for certain fluids and needs temperature dependency.

Further, the modeling approach was studied with the Soave-Redlich-Kwong (SRK) EoS using both classical and Huron-Vidal mixing rules. It was found that the SRK based models can also predict the gas injection effect but the molar amount of asphaltene in C6+ fraction needs to be fixed to a certain value at which the binary injection parameters for gas/light alkanes-asphaltenes pairs are regressed.

It is shown that the modelling approach is not affected when the C6+ fraction is divided into multiple heavy and one asphaltene components instead of one heavy and one asphaltene component. Thus, it can easily be integrated with existing PVT simulators.

The models presented can predict onset conditions when different n-alkane precipitants are used. Based on experimental data of each binary system, the models can also predict the asphaltene stability when more than two crudes are blended.

Finally, a MATLAB tool was developed to calculate asphaltene phase envelope with or without gas injection and PVT properties of reservoir fluids. The software is disseminated and is used by members of the CHIGP industry Consortium.



*Oil-Gas Separator System.*



# Thermal Simulation of Flow in Heavy Oil Reservoirs



**Duncan Paterson, PhD.**  
Currently postdoc at CERE

Full title:  
**"Flash Computation and EoS Modelling for Compositional Thermal Simulation of Flow in Porous Media".**

Supervisors:  
**Wei Yan, Erling H. Stenby, Michael Michelsen.**

The project was funded by ExxonMobil and by ConocoPhillips.

Of the total known world oil reserves only 30 % are conventional sources, while 70 % are heavy oil, extra heavy oil, oil sands and bitumen. Presently, the cost of producing heavy oil is often close to the sale price of the oil. Therefore, the cost of production needs to come down. To that end, better understanding of the production processes is required. The focus of the project is thermodynamic description of the oil.

Heavy oil is a viscous and dense substance, which flows very slowly under gravity at atmospheric temperature. Most often it is necessary to use steam to reduce the viscosity and enhance oil production. Production can be further enhanced with a light hydrocarbon solvent.

Simulation of heavy oil reservoirs is not trivial, as they undergo large changes in temperature and pressure depending on the applied production strategy. Furthermore, the use of a light hydrocarbon solvent can lead to highly asymmetric mixtures and the appearance of a second oleic phase.

A number of possible equations of state (EoS's) were evaluated. It was found that if the interaction between the water and hydrocarbon phases is not considered important, then the commonly used cubic EoS's with the van der Waals mixing rules are suitable. If more complex interactions are considered important, then the cubic EoS's can be used with the Huron-Vidal type mixing rules. More complex EoS's such as cubic plus association (CPA) or PC-SAFT can also be used.

For thermal simulation it is necessary to add an energy balance to the system. Commonly, the temperature is used as an additional primary variable. The resulting isothermal flash specification can lead to some problems during transient simulation. The fluid in some grid-blocks may become narrow boiling. The enthalpy of a narrow boiling mixture changes rapidly due to very small changes in temperature or pressure.

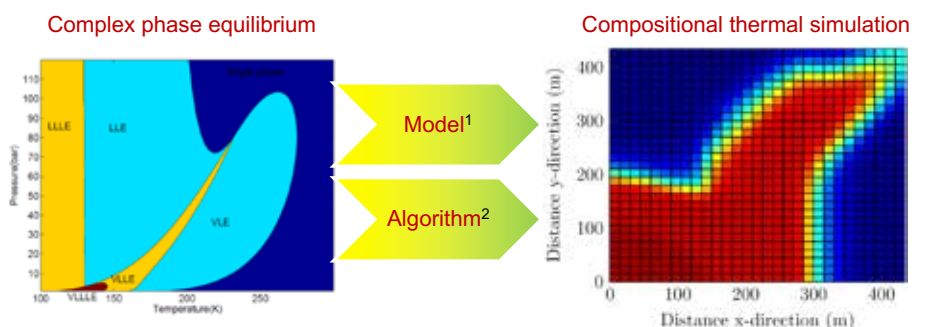
An approach using the energy directly in the flash calculation (e.g. isobaric, isenthalpic flash) is explored in this work and an algorithm presented which takes only slightly more computational resources than the conventionally used isothermal flash. This is demonstrated to be robust for a number of mixtures, and an approach

tailored for the flash calculation of mixtures containing water is described.

The conventional isothermal flash framework is cumbersome when dealing with more than two or three phases. A new method – modified RAND – is presented. The method is primarily examined for multiphase isothermal flash, with a robust implementation described. Furthermore, the conventional method of solving an EoS at a specified temperature and pressure is abandoned and a method which co-solves the EoS with the equilibrium equations is described – vol-RAND.

Finally, a thermal EoS based reservoir model is developed from an isothermal simulator. The energy balance partial differential equation is added, and the temperature used as an additional primary variable. The EoS's compared for heavy oil related fluids are implemented in the simulator. Also, a multiphase flash algorithm using modified RAND and stability analysis skipping is added to the simulator.

With the thermal reservoir simulation tool developed it is possible to carry out further comparisons and add more complexity in future work.



1. GE-type mixing rules and association models

2. Multiphase PH flash and new RAND formulations

*Handling complex equilibrium in compositional simulation through advanced thermodynamic models and efficient equilibrium calculation algorithms: The RAND-based formulations provide a new framework for multiphase flash w/ or w/o reactions.*



# Models for Deep Oil Exploration



**Farhad Varzandeh, PhD**  
Currently with Haldor  
Topsøe A/S

Full title:  
**"Modeling Study of  
High Pressure and  
High Temperature  
Reservoir Fluids".**

Supervisors:  
**Wei Yan,  
Erling H. Stenby.**

Financing was provided by  
Innovation Fund Denmark,  
Maersk Oil and DONG E&P  
as part of the NextOil  
(New Extreme Oil and Gas  
in Denmark) project.

With dwindling easily accessible oil and gas resources, the industry is driven towards deeper geological formations. In deep reservoirs, temperature and pressure can become extremely high, e.g. up to 250 °C and 2,400 bars. It is well known that established thermodynamic models have shortcomings when applied to such extreme conditions. The thesis evaluates the accuracy of existing models for HPHT (High Pressure, High Temperature) exploration, while also suggesting improvements.

HPHT reservoirs are technologically and economically risky to develop, but highly rewarding if successfully produced. A critical parameter is the length of time which equipment must withstand the HPHT conditions. Therefore, accurate knowledge of the reservoir fluid behavior is required, including density and viscosity of oil and gas at reservoir conditions. Also compressibility is critical, as compression is necessary for HPHT production.

Currently, there are neither accurate databases for these fluid properties, nor

adequate equations of state (EoSs) for density and compressibility able to predict these properties at extreme conditions. Presently, oil companies use correlations based on lower temperature and pressure databases despite their unsatisfactory predictive capability at extreme conditions – with margins of error as large as +/- 50%.

The project evaluated both cubic and non-cubic EoSs. It was found that the non-cubic models are much better than the cubics for density, compressibility, heat capacity, and Joule-Thomson coefficient calculation of both light and heavy components in reservoir fluids over a wide temperature and pressure range.

The GERG-2008 model gave the lowest deviations of all. Still, this model gave large deviations for bubble point pressure calculation on certain heavy and asymmetric binary systems, suggesting that the model may still be improved for some binary pairs.

Soave-BWR gave the closest prediction of the thermal properties to that of GERG-2008 among the other EoSs tested.

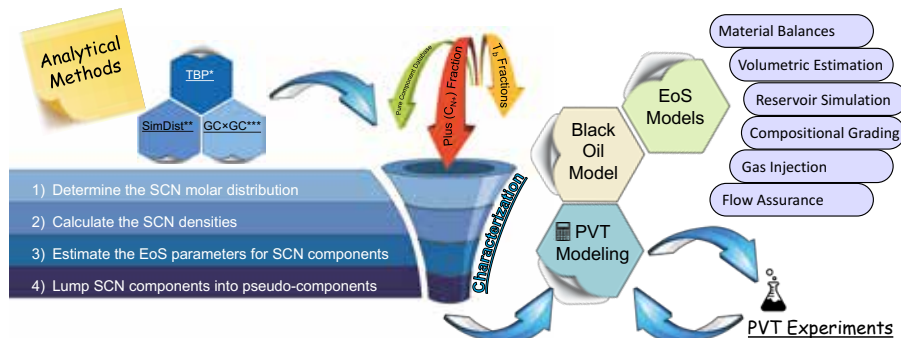
For non-cubic models like PC-SAFT, the characterization method is less mature

than cubic models. Therefore, a new reservoir fluid characterization method for PC-SAFT is proposed. In addition, this method was improved by adjusting the correlations with a large PVT database.

Importantly, a general approach to characterizing reservoir fluids for any EoS has been established. The approach consists in developing correlations of model parameters first with a database for well-defined components and the adjusting the correlations with a large PVT database. It is shown that this approach can be applied to PC-SAFT, and to classical cubic models like SRK and PR.

With the developed methods, a comparison in PVT calculation involving 17 EoS-characterization combinations and 260 reservoir fluids was made.

Finally, several new sets of mixing rules were developed for Soave-BWR for mixture calculation to improve the value of this model. It was shown that some problems with the original Soave-BWR can be fixed by the new mixing rules. However, the overall performance was not significantly improved. Development of mixing rules for non-cubic EoS models is still a semi-empirical process, requiring extensive testing.



*In addition to non-cubic EoS models, advanced characterization of heavy fractions is crucial to HPHT PVT modelling.*



# Simulation of Production from Shale

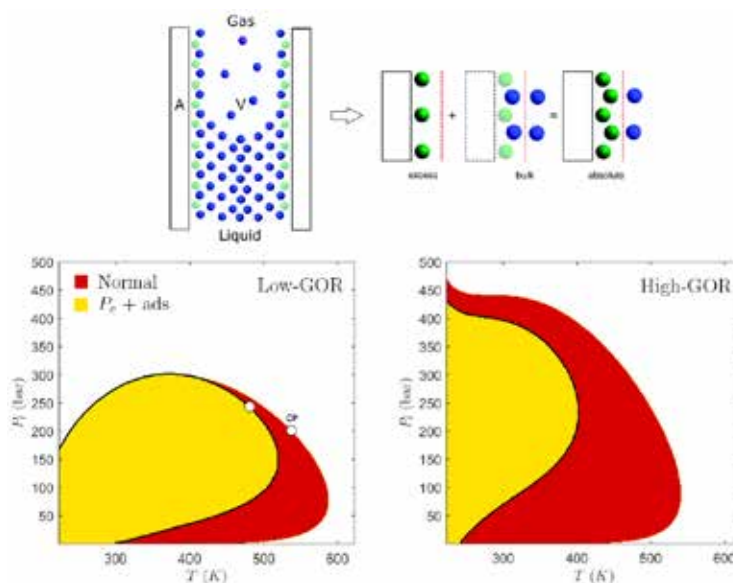


**Diego Sandoval, PhD.**  
Currently postdoc at CERE

Full title:  
**"Phase Equilibrium Modeling for Shale Production Simulation"**

Supervisors:  
**Wei Yan,**  
**Michael L. Michelsen,**  
**Erling H. Stenby.**

The project was funded by ConocoPhillips and by ExxonMobil.



*Effect of capillary pressure and adsorption on phase equilibrium of fluids with different GORs (gas oil ratios)*

Production of oil and gas from shale reservoirs has become a reality over the past few decades. As shale reservoirs are much tighter than conventional reservoirs, with pore sizes ranging in the nanometer scale, they were previously considered technically unviable to produce. New technologies such as horizontal drilling and multistage fracturing have changed the scene, but forecasting of the production remains a challenging task. The project presents models and algorithms for the purpose.

Especially in USA, production from shale has grown fast and partly substituted electricity from coal-fired power plants. However, current recovery factors are low ranging from 20-30 % for shale gas and 3-7 % for shale oil. A better understanding of the processes involved is likely to lead to higher recovery factors.

The confined nature of shale reservoirs introduces challenges in the understanding of the fluid phase behavior. High capillary forces can be experienced between the

liquid and vapor, and selective adsorption of components onto the rock becomes relevant.

The project presents an efficient algorithm for phase envelope calculations in the presence of capillary pressure. It is used to analyze the main changes on the phase boundary for several fluids of interest. The results show changes in the saturation pressure and temperature along the phase envelope, except at the critical point. A linear analysis explains such changes. As a result, useful mathematical relationships that estimate the magnitude of these changes were obtained. Moreover, a flash algorithm that accounts for capillarity was developed.

Since capillary pressure and adsorption occur simultaneously in shale, its combined effect was studied. A model comparison for high-pressure adsorption in shale is presented. As adsorption data in shale are scarce, additional capabilities besides the accuracy were considered. The multicomponent potential theory

of adsorption yields the best results. Moreover, it is useful to extrapolate adsorption data for hydrocarbons that are not available in the literature. An algorithm for phase split calculations considering both capillary pressure and adsorption was developed. The results show that adsorption and capillary pressure can significantly change the phase behavior. In general, a shrunk phase envelope with a shifted critical point is obtained for hydrocarbon mixtures. This behavior is mainly caused by compositional changes in the bulk phase due to selective adsorption of the heavier components onto the rock, while the change in bubble point pressure is mainly due to capillary pressure.

In conclusion, the project has developed several robust calculation tools for phase equilibrium in porous media with capillary pressure and adsorption effects. Analysis based on use of these tools shows capillary pressure and adsorption to have non-negligible effects on phase equilibrium in shale.



# Promotion of Hydrates for Carbon Capture



**Fragkiskos Tzirakis,  
PhD**

Currently postdoc at  
University of Thessaloniki,  
Greece

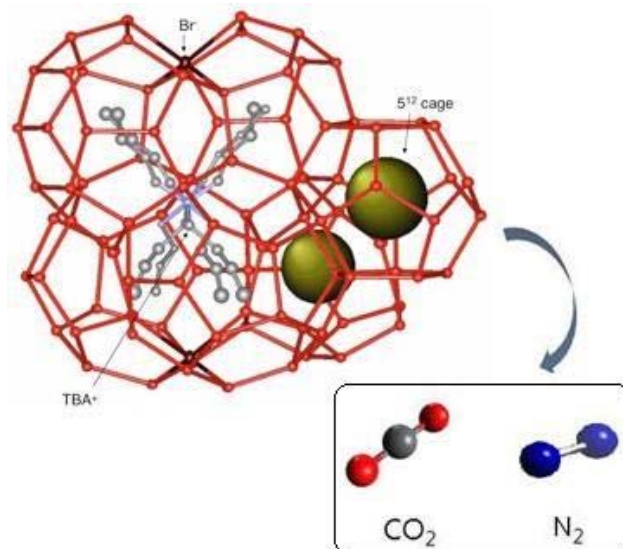
Full title:

**"An Experimental and  
Theoretical Study of  
CO<sub>2</sub> Hydrate Formation  
Systems".**

Supervisors:

**Georgios Kontogeorgis,  
Nicolas von Solms,  
and from France:  
Christophe Coquelet  
and Paolo Stringari.**

The project was sponsored  
by the Danish Technical  
Research Council (FTP) and  
included a 7 month stay at  
MINES ParisTech, France.



Carbon Capture and Storage (CCS) has received increasing heed over the last decades as a method for limiting carbon dioxide (CO<sub>2</sub>) emissions of flue gas from power and process plants. Gas hydrate crystallization has been proposed as a technique for post-combustion capture of CO<sub>2</sub>. The project demonstrates how hydrate formation can be chemically promoted.

Gas hydrates are crystalline solids composed of water and gas. During formation, gas molecules are captured in water cavities consisting of hydrogen-bonded water molecules.

In carbon capture, gas hydrates are highly specific, capturing only the CO<sub>2</sub>. This is an obvious advantage. The drawback is that flue gas has poor conditions for hydrate formation. In nature, hydrates are formed at low temperature and quite high pressure. Flue gas normally has the adverse characteristics. The flue gas could be cooled and/or pressurized for the purpose, but that would be very costly. Instead, hydrate formation can be promoted chemically.

The thesis investigates a range of hydrate promoters including tetra-n-butyl ammonium bromide (TBAB), tetra-n-butylammonium fluoride (TBAF), cyclopentane (CP), and mixtures of TBAB and TBAF with CP.

The study revealed that simultaneous use of these chemicals achieved greater pressure reduction than if they were used separately.

The use of higher TBAB concentration (1.38 mol%) and CP (5 vol%) revealed a promotion effect and as the pressure increases (>3.5 MPa), the effect increases. In addition, the higher the CO<sub>2</sub> concentration, the stronger the promotion is for every TBAB solution.

In the project, a substantial amount of new experimental data was produced mainly targeted on pressure-temperature (PT) measurements. A further ambition was to develop a theoretical framework in relation to both hydrate inhibition in oil and gas industry and hydrate promotion in CO<sub>2</sub>

capture. A model previously developed at CERE based on the van der Waals and Platteeuw hydrate model was used. This model describes the solid hydrate phase. It is typically combined with a Cubic-Plus-Association (CPA) equation of state and an activity coefficient model for description of the co-existing fluid phases.

The model very satisfactorily predicted the CP results from the project and also other CO<sub>2</sub> + cyclohexane hydrate results from literature. The model's consistency relies on fluid phases being modeled only with CPA EoS while correlations are utilized in current publications for the aqueous phase and an EoS for the hydrate phase.

In conclusion, both the experimental data and theoretical developments in the project will contribute to shedding light on the impact and usefulness of potential hydrate promoters.



# **Research Funding 2017**



# Research Funding 2017

As a university research center our objective is to spend all of our money on research. No management bonuses or other 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 Postdoc level.

The research carried out in CERE is funded by grants from a number of public and private sponsors. The external funding received in 2017 fell under the following projects and categories (all amounts in kEUR):



**Total external funding (kEUR)**



PHD DTU

**533**

BIOCO<sub>2</sub>

**386**

DHRTC

**880**

OTHER  
PRIVATE

**333**

OTHER  
PUBLIC

**240**

INNOVATIONS-  
FOND

**640**



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**3,852**

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## Faculty



**Ida Lykke Fabricius**  
DTU Civil Engineering



**Georgios Kontogeorgis,**  
DTU Chemical Engineering



**Michael L. Michelsen,**  
DTU Chemical Engineering  
Emeritus



**Alexander A. Shapiro,**  
DTU Chemical Engineering



**Nicolas von Solms,**  
DTU Chemical Engineering



**Erling H. Stenby,**  
DTU Chemistry



**Kaj Thomsen,**  
DTU Chemical Engineering



**John Bagterp,**  
DTU Compute



**Philip L. Fosbøl,**  
DTU Chemical Engineering



**Wei Yan,**  
DTU Chemistry



**Katrine Alling Andreassen,**  
DTU Civil Engineering



**Arne Døssing,**  
DTU Space



**Xiaodong Liang,**  
DTU Chemical Engineering



**Allan P. Engsig Karup,**  
DTU Compute



**Thomas G. Petersen,**  
DTU Civil Engineering

## Associated faculty



**Klaus Mosegaard,**  
Niels Bohr Institute



### Scientific Staff

Teresa Regueira Muniz,  
DTU Chemistry

Liang Mu,  
DTU Chemical Engineering

Maria del Pilar C. Vidal,  
DTU Civil Engineering

Nikolaj Blom,  
DTU Chemical Engineering

Karen Guldbæk Schmidt,  
DTU Civil Engineering

Waseem Arshad,  
DTU Chemical Engineering

Alay Arya,  
DTU Chemical Engineering

Luydmilla Geer,  
DTU Chemical Engineering

Susana Almeida,  
DTU Chemical Engineering

Carsten Völker,  
DTU Compute

Duncan Paterson,  
DTU Chemistry

Diego Sandaval,  
DTU Chemistry

Torsten Stilling,  
DTU Chemical Engineering

Jyoti Shanker Pandey,  
DTU Chemical Engineering

Anders Schlaikjer,  
DTU Chemical Engineering

Ivanka Orozova-Bekkevold,  
DTU Civil Engineering

Xiaoyan Liu,  
DTU Chemistry

### Technical and Administrative Staff

Povl Valdemar Andersen,  
DTU Chemical Engineering

Anne Louise Biede,  
DTU Chemical Engineering

Christian Carlsson,  
DTU Chemical Engineering

Thoung Dang,  
DTU Chemical Engineering

Duc Thuong Vu,  
DTU Chemical Engineering

Hector Ampuero Diaz,  
DTU Environment

Sinh Hy Nguyen,  
DTU Environment

John Troelsen,  
DTU Civil Engineering

Zacarias Tecle,  
DTU Chemical Engineering

Patricia Wagner,  
DTU Chemical Engineering

Hanne Pernille Andersen,  
DTU Chemical Engineering

### PhD Students

Lisa Pasquinelli,  
DTU Civil Engineering

Carolina Figueroa,  
DTU Chemical Engineering

Susana Almeida,  
DTU Chemical Engineering

Anders Schlaikjer,  
DTU Chemical Engineering

Tobias Orlander,  
DTU Civil Engineering

Duncan Paterson,  
DTU Chemistry

Casper Schytte Hemmingsen,  
DTU Mechanics

Christos Tsanas,  
DTU Chemistry

Sarouyeh Khoshkolgh, Niels Bohr Institute

Henrik Lund Nielsen,  
DTU Chemical Engineering

Justin Brand,  
DTU Chemical Engineering

Andre Pinto Vinhal,  
DTU Chemical Engineering

Lasse Hjuler Christiansen,  
DTU Compute

Tobias Ritchel,  
DTU Compute

Xianglei Meng,  
DTU Chemical Engineering

Steen Hørsholt,  
DTU Compute

Leonardo Meireles,  
DTU Civil Engineering

Francois Kruger,  
DTU Chemical Engineering

Mauro Torli,  
DTU Chemical Engineering

Li Sun,  
DTU Chemical Engineering

Laura Paci,  
DTU Civil Engineering

Einer Madsen Storebø,  
DTU Civil Engineering

Yingjun Cai,  
DTU Chemical Engineering

Yigun Liu,  
DTU Chemistry

Petter Lomsøy,  
DTU Chemical Engineering

Edgar Camacho,  
DTU Chemical Engineering

### External PhD Students

Maria Gundersen Deslauriers,  
DTU Chemical Engineering

Xinyan Liu,  
DTU Chemical Engineering

Spardha Virendra Jhamb,  
DTU Chemical Engineering

Mirhossein Taherioghtagsara,  
DHRTC

Jiasheng Hao,  
DHRTC

Yanrong Liu,  
DTU Chemistry

Olivia Ana Perederic,  
DTU Chemical Engineering

### External / Associated Staff

Irene Rocchi,  
DTU Civil Engineering

Jens Honore Walther,  
DTU Mechanics

### Guests

Asma Rafsanjani,  
DTU Chemical Engineering

Samira Mohammadkhani,  
DTU Chemical Engineering

Kai Kang,  
DTU Chemical Engineering


Rafael Tini,  
DTU Chemical Engineering

### Student Workers

Niels Frithjof Lanholdt

Roman Birka





### **Electronic Version of the CERE Annual Report 2017**

This printed report is a concentrated version of the CERE Annual Report 2017. The full report is found in a PDF version at CERE's website [www.cere.dtu.dk](http://www.cere.dtu.dk)

The e-report has additional content which is not present in the printed report:

#### **Publications in 2017**

CERE performs well in the world of energy resources engineering. This is reflected in the publications produced every year. The full list of 2017 publications is found in the e-report.

#### **Conference Contributions & Invited Speakers**

The full list of conference contributions from CERE's researchers is found in the e-report.

#### **Master's Theses**

The list of 2017 Master's Theses is found in the e-report.