

CERE

ANNUAL
REPORT 2017

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

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.

CERE Annual Report 2017

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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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the energy sector
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but also invites new
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two of the many
highlights in the
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PhD Theses of the Year

Main results from
the PhD projects
concluded during
the year – seven in
all – are presented.

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 Guldberg 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 CO₂, oil, gas, and water

In this report, you will see that we continue to focus on various dimensions of CO₂: capture, transport, utilization and storage. The CO₂ oriented projects include the EU-funded INTERACT project on CO₂ capture using enzyme-based solvents in collaboration with Novozymes. Further, a recently completed project on gas hydrates use for CO₂ capture in collaboration with MINES ParisTech in France. Also, the recently started BioCO₂ project on turning

CO₂ 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 CO₂.

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

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
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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 CO₂ for industrial purposes, capture and storage of CO₂, 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

Hess Danmark ApS, Denmark

KBC, United Kingdom
- Linde AG, Germany

Maersk Oil, Denmark

MOL, Hungary

National Oilwell Varco, USA

Petrobras S.A., Brazil

Schlumberger, USA

Shell Global Solutions International B.V., The Netherlands

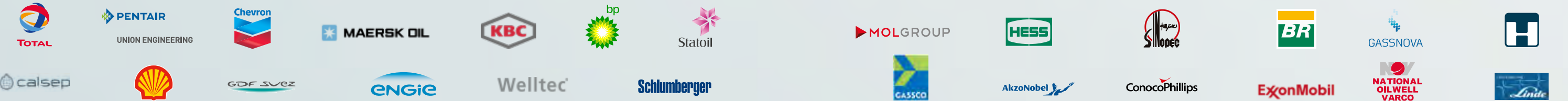
SINOPEC, P.R. China

Statoil, Norway

Total, France

Union Engineering, Denmark

Welltec, Denmark



From the left: Eirini Karakatsani, Thermodynamics Specialist at Topsoe; Monzurul Alam, Reservoir Geomechanics Engineer at Schlumberger; Jacob Sonne, Principal Engieer 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 CO₂ pressures. This demand is driven partly by high pressure reservoirs with a high CO₂ content and partly by a growing interest in injection of CO₂-rich fluids into reservoirs. This has spurred a current cooperation with CERE researchers,” explains Dr. Jacob Sonne, NOV Flexibles.

Permeation of CO₂ 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 CO₂ 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 CO₂ for industrial purposes, capture and storage of CO₂, 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 Thorikild 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 CO₂ 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 CO₂ 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 CO₂ 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 CO₂ 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 CO₂ is produced. This CO₂ 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 CO₂ 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.”



Nicolas von Solms,,
Associate Professor



John Woodley,
Professor



Arne Gladis,
PhD student
(completed in 2017)

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.

CO₂ is better than its Reputation

A joint industry project led by CERE will turn an overlooked resource, CO₂ from biogas upgrading plants, into a high-value product.



“In relation to upgrading of biogas to methane, CO₂ is seen as a mere waste product and is just released into the atmosphere. But at the same time, we import CO₂ 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 BioCO₂ project.

While mainly associated with climate change, CO₂ 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 CO₂ 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, CO₂ is produced as a by-product. Roughly 35 % of the biogas is CO₂.

“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 CO₂ 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 CO₂ purity is required
Unfortunately, it is not possible to use the CO₂ from biogas upgrading directly for the various industrial purposes where

CO₂ is in demand. If things were that simple, utilization of this CO₂ 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 BioCO₂.

Besides CERE and DGC, Pentair is a partner to the project. The company specializes in plants for amine-based capture of CO₂.

“As Union Engineering, we were world leading in amine-based CO₂ 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 CO₂ 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 BioCO₂ 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 BioCO₂ 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 BioCO₂ 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 CO₂ is the main focus

of BioCO₂, the upgrading of biogas into methane is also revisited.

“Developing a better way to produce CO₂ 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 BioCO₂ 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

BioCO₂ 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 CO₂, he stresses that BioCO₂ 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, BioCO₂ 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.

“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 CO₂

Nature has vast amounts of methane stored inside so-called gas hydrates. Humankind has too much CO₂. The idea of a new project at CERE is to swap our CO₂ for methane. Specifically, the CO₂ 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 CO₂ or gas mixtures containing CO₂, 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. CO₂ can act as an agent, which drives the methane out. If the process is designed smartly, the CO₂ 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 “CO₂ impact on corrosion product (FeCO₃) 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 CO₂

reacting with steel, producing a solid corrosion product, FeCO₃. 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 FeCO₃ is a key property. A way to predict corrosion is to use existing solubility data for FeCO₃ 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 FeCO₃ 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 FeCO₃ 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 CO₂ 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 CO₂ 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 CO₂ 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 CO₂. Eventually, we will probably need both carbon capture and atmospheric cleaning to reach negative CO₂-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.



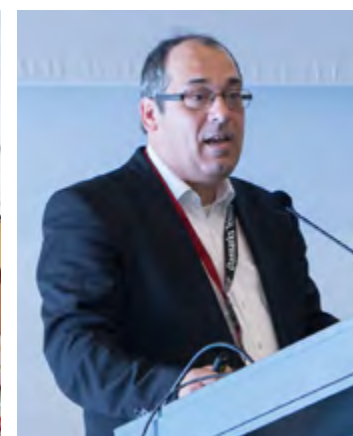
Plenary Lectures in China and Brazil

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 ConocoPhilips.

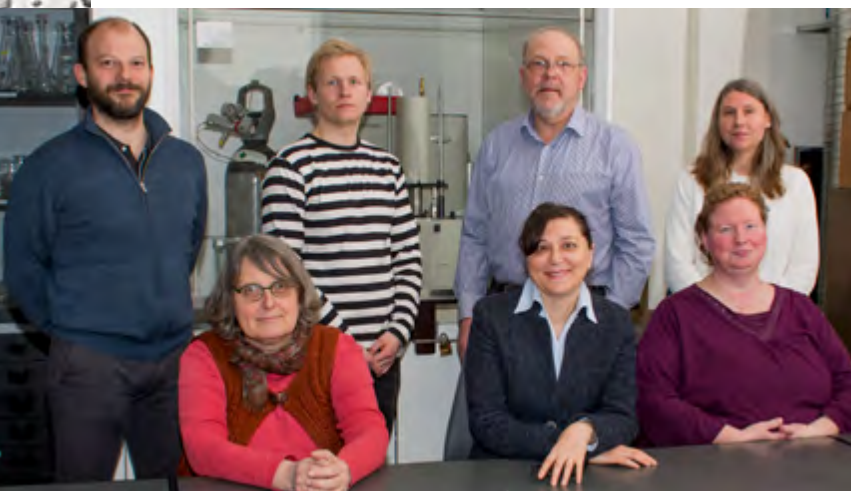
The gas may not only be injected into the reservoir, but also liberated from the oil, as the reservoir pressure decreases. Such gas may appear in the form of bubbles, plugging the porous medium and decreasing productivity of the wells. On the other hand, the liberated gas might flow up in the reservoir 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 years' 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 years' 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 CO₂ 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 CO₂ 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

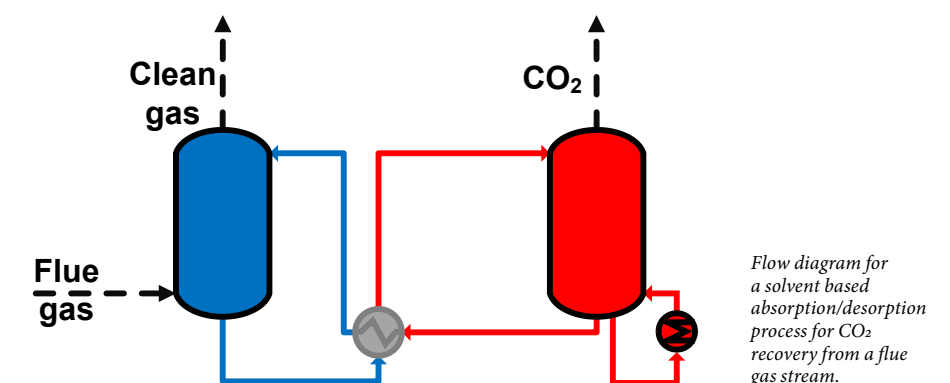
obstacle for industrial implementation. This project suggests that enzymes can be used as kinetic rate promoters that enhance the mass transfer of CO₂ with slow-capturing but energetically favorable solvents. Specifically, the enzyme carbonic anhydrase (CA), which enhances the mass transfer of CO₂ in our lungs by catalyzing the reversible hydration of CO₂, 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 CO₂ capture. The model accurately describes the CO₂ 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 CO₂ 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 CAPCO₂ 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 CO₂
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.

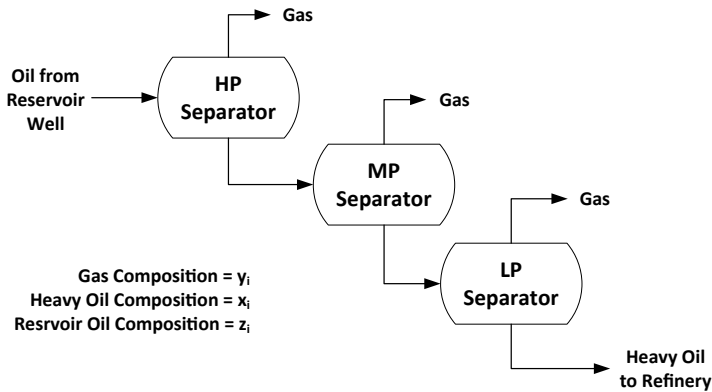
The developed approach using both CPA and PC-SAFT EoS's was compared with the literature approach based on the PC-SAFT EoS. It was found that the PC SAFT model cannot correlate the asphaltene upper onset pressure boundary for certain fluids and needs temperature dependency.

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.

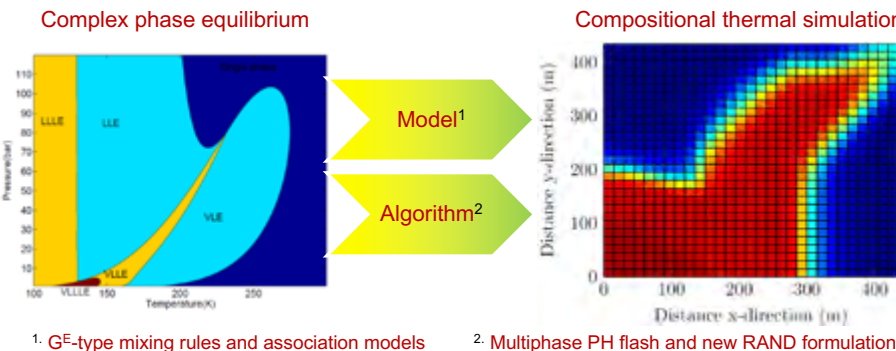
An approach using the energy directly in the flash calculation (e.g. isobaric, isenthalpic flash) is explored in this work and an algorithm presented which takes only slightly more computational resources than the conventionally used isothermal flash. This is demonstrated to be robust for a number of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

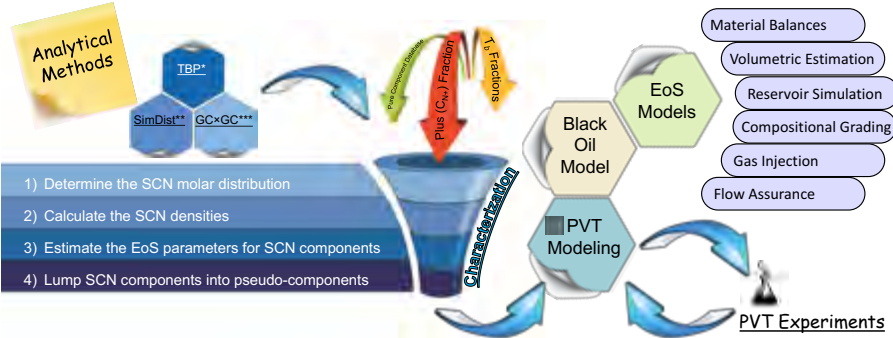
For non-cubic models like PC-SAFT, the characterization method is less mature

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

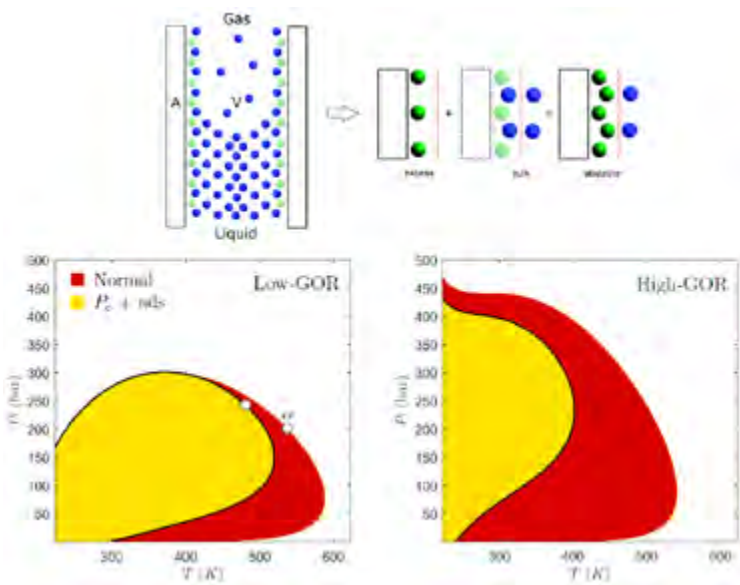


Diego Sandoval, PhD.
Currently postdoc at CERE

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

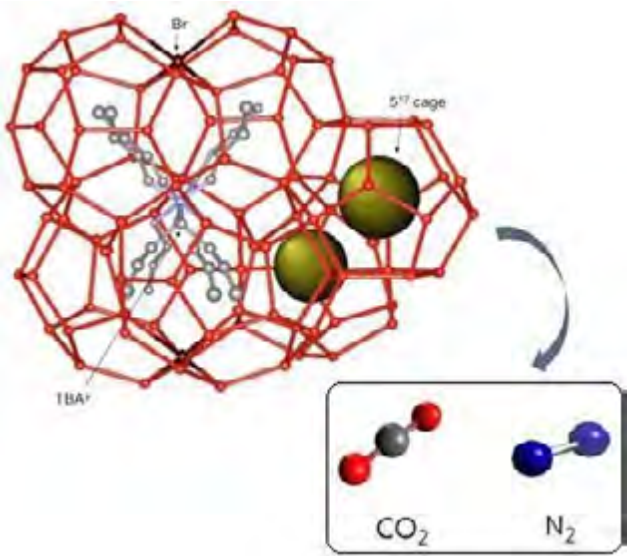


Fragkiskos Tzirakis, PhD
Currently postdoc at University of Thessaloniki, Greece

Full title:
“An Experimental and Theoretical Study of CO₂ 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 (CO₂) emissions of flue gas from power and process plants. Gas hydrate crystallization has been proposed as a technique for post-combustion capture of CO₂. 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 CO₂. 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 CO₂ 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 CO₂

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 CO₂ + 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.

Conference Contributions

FEBRUARY

SPE Reservoir Simulation Conference, Montgomery, Texas, USA, 20-22 Feb 2017

D. Paterson, M.L. Michelsen, E.H. Stenby, and W. Yan, “New Formulations for Isothermal Multiphase Flash”, SPE Reservoir Simulation Conference, Montgomery, Texas, USA, 20-22 Feb 2017 (oral)

APRIL

East Meets West (EMW), Cracow, Poland, 4-7 April, 2017

Y. Liu, A.A. Wibowo, T. Regueira, E.H. Stenby, and W. Yan, “PVT study of model reservoir fluids at HPHT conditions”, East Meets West (EMW), Cracow, Poland, 4-7 April, 2017 (poster)

IOR NORWAY 2017 – 19th European Symposium on Improved Oil Recovery, Stavanger, Norway, 24-27 April, 2017

T. Voake, A. Nermoen, R.I. Korsnes, and I.L. Fabricius, “Induced Shear Failure by Temperature Reduction at Uni-axial Strain Conditions”, IOR NORWAY 2017 – 19th European Symposium on Improved Oil Recovery, Stavanger, Norway, 24-27 April 2017 (poster) - Extended abstract 11p.

MAY

9th International Conference on Porous Media & Annual Meeting, Rotterdam, Netherlands; 8-11 May, 2017

I.L. Fabricius, M.M. Alam, A. Alexeev, K.H. Chakravarty, P.L. Fosbøl, K. Katika, and A. Shapiro, “Flooding of North Sea chalk and greensand cores with specific brines”, 9th International Conference on Porous Media & Annual Meeting, Rotterdam, Netherlands, May 8-11, 2017 (oral) - Abstract 2p.

SAFT 2017, Heidelberg, Germany, 11-13 May, 2017

X. Liang, M.L. Michelsen, and G.M. Kontogeorgis, “Density gradient theory for interfacial tension calculations”, SAFT 2017, Heidelberg, Germany, 11-13 May, 2017 (oral)

29th European Symposium on Applied Thermodynamics (ESAT), Bucharest, Romania, 18-21 May 2017

F.J. Kruger, G.M. Kontogeorgis, and N. von Solms, “A new association scheme and CPA parameterization of monoethylene glycol”, 29th European Symposium on Applied Thermodynamics (ESAT), Bucharest, Romania, 18-21 May 2017 (oral)

F.J. Kruger, G.M. Kontogeorgis, and N. von Solms, “Evaluation of Cubic-Plus-Association parameterization for monoethylene glycol”, 29th European Symposium on Applied Thermodynamics (ESAT), Bucharest, Romania, 18-21 May 2017 (poster)

A. Schlaikjer, K. Thomsen, and G.M. Kontogeorgis, “Ion-specific electrolyte CPA for aqueous single- and multiple salt solutions”, 29th European Symposium on Applied Thermodynamics (ESAT), Bucharest, Romania, 18-21 May, 2017 (oral)

A.P.C.M. Vinhal, G.M. Kontogeorgis, and W. Yan, “An engineering perspective of a crossover equation of state”, 29th European Symposium on Applied Thermodynamics (ESAT), Bucharest, Romania, 18-21 May 2017 (oral)

C. Tsanas, E.H. Stenby, and W. Yan, “Calculation of Multiphase Chemical Equilibrium by Non-Stoichiometric Methods”, 29th European Symposium on Applied Thermodynamics (ESAT), Bucharest, Romania, 18-21 May 2017 (oral)

C. Tsanas, E.H. Stenby, and W. Yan, “Phase Equilibrium Modeling for the DME Enhanced

Water-flooding”, 29th European Symposium on Applied Thermodynamics (ESAT), Bucharest, Romania, 18-21 May 2017 (poster)

D. Paterson, M.L. Michelsen, E.H. Stenby, and W. Yan, “General Multiphase PH Flash and Its Application in Thermal Recovery”, 29th European Symposium on Applied Thermodynamics (ESAT), Bucharest, Romania, 18-21 May 2017 (oral)

D. Paterson, M.L. Michelsen, E.H. Stenby, and W. Yan, “RAND-based Formulations for Isothermal Multiphase Flash”, 29th European Symposium on Applied Thermodynamics (ESAT), Bucharest, Romania, 18-21 May 2017 (oral)

S. Almeida, R. Lundsgaard, and N. von Solms, “Modeling and Measurement of Solubility and Swelling in Supercritical Carbon Dioxide – Polymer Systems.” 29th European Symposium on Applied Thermodynamics (ESAT), Bucharest, Romania, 18-21 May 2017 (oral)

G.M. Kontogeorgis, “Teaching chemical engineering thermodynamics at DTU: How, why, impressions and some personal thoughts”, 29th European Symposium on Applied Thermodynamics (ESAT), Bucharest, Romania, 18-21 May 2017 (Invited lecture)

G.M. Kontogeorgis, “Electrolyte thermodynamics: Current status, future challenges and some applications of an electrolyte CPA equations of state”, 29th European Symposium on Applied Thermodynamics (ESAT), Bucharest, Romania, 18-21 May 2017 (oral)

11th Panhellenic Scientific Conference of Chemical Engineering, Thessaloniki, Greece, 25-27 May, 2017

G.M. Kontogeorgis, “Thermodynamics for a sustainable chemical engineering in a changing world”, 11th Panhellenic Scientific Conference of Chemical



Engineering, Thessaloniki, Greece, 25-27 May, 2017 (invited lecture)

4th International Workshop on Rock Physics, Trondheim, Norway, 29 May-2 June, 2017

L.T.P. Meireles, M.J. Welch, and I.L. Fabricius, “Water saturation and stiffness of chalk from Halfdan and Dan fields, Danish North Sea”, 4th International Workshop on Rock Physics, Trondheim Norway, 29 May-2 June 2017, (poster) – 2 p. abstract

T. Orlander, K.D. Enemark, K.A. Andreassen, and I.L. Fabricius, “Permeability in deep North Sea sandstones as predicted from NMR”, 4th International Workshop on Rock Physics, Trondheim, Norway, 29 May-2 June 2017 (oral)

J. Regel, and K.G. Schmidt, “Prediction of stress dependency on acoustic velocity in chalk”, 4th International Workshop on Roch Physics, Trondheim, Norway, 29 May-2 June, 2017 (poster) – 2 p. abstract

JUNE

The 18th International Conference on Petroleum Phase Behavior & Fouling, PetroPhase 2017, Le Havre, France, 11-15 June, 2017

D. Sandoval, W. Yan, M.L. Michelsen, and E.H. Stenby, “Influence of adsorption and capillary pressure on phase equilibrium in shale reservoirs”, The 18th International Conference on Petroleum Phase Behavior & Fouling, PetroPhase 2017, Le Havre, France, 11-15 June, 2017 (oral)

D. Sandoval, W. Yan, E.H. Stenby, and M.L. Michelsen. “Adsorption and Capillary Pressure Influence on Phase Equilibria Inside Shale Reservoirs” PetroPhase 2017, Le Havre, 11-15 June 2017 (poster)

T. Regueira, E.H. Stenby, and W. Yan. “Density and Compressibility of Multi-component n-Alkane Mixtures up to

463 K and 140 MPa” PetroPhase 2017, Le Havre, 11-15 June 2017 (poster)

T. Regueira, C.P. Chatziagapiou, F. Varzandeh, E.H. Stenby, and W. Yan, “Heat capacity and Joule-Thomson coefficient of the binary system methane + n-decane”, PetroPhase 2017, Le Havre, 11-15 June 2017 (poster)

Mountjoy II – Carbonate Pore Systems, Texas, Austin, USA, 25-29 June, 2017

I.L. Fabricius, “Porosity in Chalk”, Mountjoy II - Carbonate Pore Systems, Texas, Austin, USA, 25-29 June, 2017 (oral key note) - Abstracts p55.

79th EAGE Conference & Exhibition 2017, Paris, France 12-15 June, 2017

L.T.P. Meireles, A. Hussain, M.J. Welch, and I.L. Fabricius, “Controls on Cementation in a Chalk Reservoir”, 79th EAGE Conference & Exhibition 2017, Paris, France, 12-15 June 2017 (oral) - Extended abstract 5p.

51st U.S. Rock Mechanics/Geomechanics Symposium, San Francisco, California, USA, 25-28 June, 2017

T. Orlander, K.A. Andreassen, and I.L. Fabricius, “Temperature effects on stiffness moduli of reservoir sandstone from the Deep North Sea”, 51st U.S. Rock Mechanics/ Geomechanics Symposium, San Francisco, California, USA, 25-28 June, 2017 (oral)

9th International Conference on Gas Hydrates, Denver, Colorado, USA, 25-30 June, 2017

F. Tzirakis, P. Stringari, N. von Solms, C. Coquelet, and G.M. Kontogeorgis, “Measurement and modelling of hydrate promotion for systems of interest in post-combustion carbon dioxide capture,” 9th International Conference on Gas Hydrates, Denver Colorado, USA 25-30 June, 2017 (poster)

L. Mu, and N. von Solms, “Methane Production and Carbon Capture by Hydrate Swapping,” 9th International Conference on Gas Hydrates, Denver Colorado, USA 25-30 June, 2017 (poster)

JULY

6th Biot Conference on Poromechanics, American Society of Civil Engineers, Paris, France, 9-13 July, 2017

I.L. Fabricius, C. Haugwitz, P.B. Larsen, and N.H. Schovsbo, “Elasticity and Density of Paleozoic Shales from Bornholm”, 6th Biot Conference on Poromechanics, American Society of Civil Engineers, Paris, France, 9-13 July, 2017 (oral) – in Poromechanics 2017 - Proceedings of the 6th Biot Conference on Poromechanics. American Society of Civil Engineers, pp. 1299-1306. DOI: 10.1061/9780784480779.161 oral

L.T.P. Meireles, M.M. Alam, and I.L. Fabricius, “Permeability Estimation in Chalk Using NMR and a Modified Kozeny Equation”, 6th Biot Conference on Poromechanics, American Society of Civil Engineers, Paris, France, 9-13 July, 2017 (poster) - in MV, PD, J-MP & SG (eds), Poromechanics VI: Proceedings of the 6th Biot Conference on Poromechanics. American Society of Civil Engineers, pp. 1208-1215. DOI: 10.1061/9780784480779.150

T. Orlander, L. Pasquinelli, J.J. Asmussen, A.A. Marczyński, E. Adamopoulou, H. Milsch, and I.L. Fabricius, “Thermal Conductivity of Sedimentary Rocks as Function of Biot’s Coefficient”, 6th Biot Conference on Poromechanics, American Society of Civil Engineers, Paris, France, 9-13 July, 2017 (oral) - in MV, PD, J-MP & SG (eds), Poromechanics VI: Proceedings of the 6th Biot Conference on Poromechanics. American Society of Civil Engineers, July 9-13 2017, pp. 1396-1404

M.K. Sørensen, and I.L. Fabricius, “How Pore Filling Shale Affects Elastic Wave Velocities in Fully and Partially Saturated Sandstone: Characterization, Measurement, and Modelling”, 6th Biot Conference on Poromechanics, American Society of Civil Engineers, Paris, France, 9-13 July, 2017 (oral) - in MV, PD, J-MP & SG (eds), Poromechanics VI: Proceedings of the 6th Biot Conference on Poromechanics. American Society of Civil Engineers July 9-13 2017,, pp. 1714-1721. DOI: 10.1061/9780784480779.212

The 20th World Congress of the International Federation of Automatic Control, Toulouse, France, 9-14 July, 2017

T.K.S. Rischel, J. Gaspar, A. Capolei, and J.B. Jørgensen, “A thermodynamic library for simulation and optimization of dynamic processes”, The 20th World Congress of the International Federation of Automatic Control, Toulouse, France, 9-14 July, 2017 (oral) - Published in IFAC-PapersOnLine (proceedings) on ScienceDirect: <https://www.sciencedirect.com/science/article/pii/S2405896317314234>

A. Capolei, L.H. Christiansen, and J.B. Jørgensen, “Offset risk minimization for open-loop optimal control of oil reservoirs”, The 20th World Congress of the International Federation of Automatic Control, Toulouse, France, 9-14 July, 2017 (oral) - ProciFAC-PapersOnline, vol. 50, Issue 1, pages 10620-10625

AUGUST

8th International Workshop on Natural Energies (IWONE), Höör, Sweden, 4-6 August, 2017

N.S. Blom, “Using new media to communicate water research and quantum biology”, 8th International Workshop on Natural Energies (IWONE), Höör, Sweden, 4-6 August, 2017 (oral) - <http://www.iet-community.org/iwone/IWONE8/presentations.html>

S.H. Ingwersen, H.M. Kristensen, R.B. Jensen, A. Heerfordt, and N.S. Blom, "Controlled experiments with vortexed water in agriculture", 8th International Workshop on Natural Energies (IWONE), Höör, Sweden, 4-6 August, 2017 (oral) - <http://www.iet-community.org/iwone/IWONE8/presentations.html>

SEPTEMBER

NEAR SURFACE Geoscience 2017, Malmö, Sweden, 3-7 September, 2017

H.D.H. Holmslykke, C. Kjøller, and I.L. Fabricius, "Seasonal Deep Aquifer Thermal Energy Storage in the Gassum Sandstone Formation" NEAR SURFACE Geoscience 2017 3-7 September 2017, Malmö, Sweden. Extended abstract 5p. co-author

Thermodynamics 2017, Edinburgh, Scotland, 5-8 September 2017

D. Paterson, M.L. Michelsen, E.H. Stenby, W. Yan. "Extension of Modified RAND to Other State Function Based Flash Specifications", Thermodynamics 2017, Edinburgh, Scotland, 5-8 September 2017 (poster)

G.M. Kontogeorgis, "Recent advances with association theories", Thermodynamics 2017, Edinburgh, Scotland, 5-8 September 2017 (oral)

IEA-EOR 2017, 38th Annual Workshop & Symposium, Riviera Maya, Mexico, 26-30 September, 2017

D. Paterson, C. Tsanas, M.L. Michelsen, E.H. Stenby, W. Yan. "New Framework for Multiphase Flash in Compositional Simulation", 38th Annual Workshop & Symposium, IEA-EOR 2017, Riviera Maya, Mexico, 26-30 September 2017 (poster)

2017 Chinese Academy of Sciences-The World Academy of Sciences for the

Advancement of Science in Developing Countries: Symposium on Green Chemistry and Technology for Sustainable Development (GCT2017), Beijing, China, 4-6 September, 2017

N. von Solms, "Transition to a fossil-free energy landscape - Greener solutions for gas production and carbon capture and storage," 2017 Chinese Academy of Sciences-The World Academy of Sciences for Advancement of Science in Developing Countries: Symposium on Green Chemistry and Technology for Sustainable Development (GCT2017), Beijing, China, September 4-6, 2017

OCTOBER

10th World Congress of Chemical Engineering, Barcelona, Spain, 1-5 October, 2017

A. Vinhal, G.M. Kontogeorgis, and W. Yan, "A crossover approach for the Cubic-Plus-Association Equation of State", 10th World Congress of Chemical Engineering, Barcelona, Spain, 1-5 October, 2017 (oral)

The 27th European Symposium on Computer Aided Process Engineering, Barcelona, Spain, 1-5 October, 2017

T.K.S. Ritschel, A. Capolei, and J.B. Jørgensen, "The adjoint method for gradient-based dynamic optimization of UV flash processes", The 27th European Symposium on Computer Aided Process Engineering, Barcelona, Spain, 1-5 October, 2017 (poster) - Published in Computer Aided Chemical Engineering (proceedings) on ScienceDirect: <https://www.sciencedirect.com/science/article/pii/B9780444639653503470>

A. Capolei, L.H. Christiansen, and J.B. Jørgensen, "A novel approach for risk minimization in life-cycle oil production optimization", The 27th European

Symposium on Computer Aided Process Engineering, Barcelona, Spain, 1-5 October, 2017 (oral) - Published in Computer Aided Chemical Engineering (proceedings) on ScienceDirect: <https://www.sciencedirect.com/science/article/pii/B9780444639653500283>

SPE 3rd Kuwait Oil & Gas Show and Conference, Kuwait City, Kuwait, 15-18 October, 2017

M.W. Arshad, P.L. Fosbøl, A. Shapiro, and K. Thomsen, "Water-Oil emulsions with fines in smart water enhanced oil recovery", SPE 3rd Kuwait Oil & Gas Show and Conference, Kuwait City, Kuwait, 15-18 October, 2017 (poster (e-poster), OnePetro (www.onepetro.org) Paper number: SPE-187620-MS.

IX Brazilian Conference on Thermodynamics and V School of Thermodynamics (CBTermo 2017), Porto Alegre, Brazil, 23-27 October, 2017

G. Kontogeorgis, "Equations of state in three centuries – Are we closer to arriving to a single model for all applications?", IX Brazilian Conference on Thermodynamics and V School of Thermodynamics (CBTermo 2017), Porto Alegre, Brazil, 23-27 October, 2017 (Invited lecture)

12th Annual Conference on the Physics, Chemistry and Biology of Water, Sofia, Bulgaria, 26-29 October, 2017

N.S. Blom, "Using new media to communicate water research and quantum biology", 12th Annual Conference on the Physics, Chemistry and Biology of Water, Sofia, Bulgaria, 26-29 October, 2017 (poster) - <http://www.waterconf.org/participants-materials/2017/posters/BlomAbs>.

Master Theses 2017

Amin Abouardini

"A feasibility study of hydrocarbon gas injection in Skjold Field"

Narjes Baqerian Dehkordi

"Wellbore stability of geothermal wells"

Kai Gao

"Direct conversion of cellulose into sorbitol by ionic liquids"

Wael Fadi Al-Masri

"Carbon dioxide injection in North Sea reservoir"

Daniel Lohne Edvardsen

"Differences between water- and oil-based drilling fluids with focus on practical aspects of borehole stability"

Maria-Lito Glykioti

"Density and heat capacity measurement of reservoir fluid related systems at high pressure

Alejandro Luis Caballero Arcos

"Reservoir-well interaction"

Tove Anne E. Ekdahl

"Petrophysics of organic rich chalk from Sheohela Basin

Niklas Flink Hansen

"Thermodynamic analysis of oil field scale and corrosion"

Casper Mølby Berg

"A feasibility study of hydrocarbon gas injection in Skjold Field"

Kasper Dupont Enemark

"Petrophysical characterization of sedimentary rocks from the deep North sea basin

Adam Stanislaw Kazmierczak

"Modelling of rock breaking under cutting and confined conditions"

Mark Bülow

"Further development and investigations of the electrolyte CPA equation of state"

Sjúrdur Jóhan Ferjá

"Permeability of opal bearing Miocene sediments"

Krystian Grzegorz Klepczyk

"Gas re-injection in North Sea reservoirs"

Laura Camila Vargas Castillo

"Concentration of highly charged industrial wastewater sources using forward osmosis - from laboratory scale to pilot scale"

Joachim Christian Franch

"Tensile strength of chalk as a function of fluid saturation"

Nomikh Kottaki

"PVT study of reservoir fluids at HPHT conditions"



Petter Lomsøy “Experimental determination of the solubility of scale minerals at high pressures and high temperatures”	Petur Sjúrdaberg “Temperature dependent elasticity of hot-water-flushed sandstone from Gassum formation”
Wojciech Jan Lopuszko “Elasticity and cementation of Cenozoic shale from the North sea”	Torsten Stilling “Thermodynamic modelling and heat integration simulation of CO ₂ compression and liquefaction for EOR”
Jyoti Shanker Pandey “Innovative techniques for Matrix acidizing in tight carbonate formations, minimizing damage to equipment and environment”	Einar Madsen Storebø “Mechanical properties of organic rich chalk from Shephela Basin”
Christos Papaspyrou “Carbon dioxide injection in North Sea reservoir”	Olimpia Seta “Measurements and correlation of PVT properties for biogas upgrading CO ₂ removal technologies”, (PLF)
Christian Sørensen Price “Investigation of the kinetics of scale formation”	Stefano Tagliaferri “Surface phenomena under s mart waterflooding”
Christine Ravnås “Petrophysical properties of heat treated chalk”	Camilo Eduardo Leiva Tellez “Small-scale anisotropic stiffness of rocks”

Publications



CERE Publications - Published in 2017

CERE 1607	<i>“Evaluation of Equations of State for Simultaneous Representation of Phase Equilibrium and Critical Phenomena”</i> Andre P.C.M. Vinhal, Wei Yan, and Georgios M. Kontogeorgis (Fluid Phase Equilibria, 437 (2017) 140-154)	CERE 1625	<i>“Modeling of Asphaltene Precipitation from Crude Oil with the Cubic Plus Association Equation of State”</i> Alay Arya, Xiaodong Liang, Nicolas von Solms, and Georgios M. Kontogeorgis (Energy and Fuels, 31 (2017) 2063-2075)
CERE 1615	<i>“Simultaneous Description of Activity Coefficients and Solubility with eCPA”</i> Anders Schlaikjer, Kaj Thomsen, and Georgios M. Kontogeorgis (I&EC Research, 56 (2017) 1074-1089)	CERE 1627	<i>“Dimerization of Carboxylic Acids: An Equation of State Approach”</i> Ioannis Tsivintzelis, Georgios Kontogeorgis, and Costas Panayiotou (Journal of Physical Chemistry Part B: Condensed Matter, Surfaces, Interfaces & Biophysical, 121 (2017) 2153-2163)
CERE 1622	<i>”Methane Production and Carbon Capture by Hydrate Swapping”</i> Liang Mu, and Nicolas von Solms (Energy Fuels, 31 (2017) 3338-3347)	CERE 1634	<i>“CO₂ Capture with Liquid-Liquid Phase Change Solvents: A Thermodynamic Study”</i> Muhammad Waseem Arshad, Philip L. Fosbøl, Nicolas von Solms, and Kaj Thomsen (Energy Procedia, 114 (2017) 1671-1681)
CERE 1623	<i>“Influence of Temperature and Solvent Concentration on the Kinetics of the Enzyme Carbonic Anhydrase in Carbon Capture Technology”</i> Arne Gladis, Maria T. Gundersen, Philip L. Fosbøl, John M. Woodley, and Nicolas von Solms (Chemical Engineering Journal, 309 (2017) 772-786)	CERE 1639	<i>“Effective stresses and shear failure pressure from in situ Biot’s coefficient, Hejre Field, North Sea”</i> J.B. Regel, I. Orozova-Bekkevold, K.A. Andreassen, N.C. Høegh van Gilse, and I.L. Fabricius (Geophysical Prospecting, 65 (2017) 808-822)



CERE 1701	<p><i>“Clay-squirt: Local flow dispersion in shale bearing sandstones”</i></p> <p>M.K. Sørensen, and I.L. Fabricius (Geophysics, 82 (2017) MR51–MR63)</p>	CERE 1706	<p><i>“Practical enhancement factor model based on GM for multiple parallel reactions: Piperazine (PZ) CO₂ capture”</i></p> <p>J. Gaspar, and P.L. Fosbøl (Chemical Engineering Science, 158 (2017) 257-266)</p>
CERE 1702	<p><i>“Determination of Zinc Sulfide Solubility to High Temperatures”</i></p> <p>Diana Carolina Figueroa Murcia, Philip L. Fosbøl, Kaj Thomsen, and Erling H. Stenby (Journal of Solution Chemistry, 46 (2017) 1805-1817)</p>	CERE 1707	<p><i>“Data requirements and modeling for gas hydrate related mixtures and a comparison of two association models”</i></p> <p>Xiaodong Liang, Georgios Aloupis, and Georgios M. Kontogeorgis (Journal of Chemical and Engineering Data, 62 (2017) 2592-2605)</p>
CERE 1704	<p><i>“Towards the understanding of microbial metabolism in relation to microbial enhanced oil recovery”</i></p> <p>Amalia Yunity Halim, Sidsel Marie Nielsen, Kristian Fog Nielsen, and Anna Eliasson Lantz (Journal of Petroleum Science and Engineering, 149 (2017) 151-160)</p>	CERE 1708	<p><i>“Multiple shooting applied to robust reservoir control optimization including output constraints on coherent risk measures”</i></p> <p>Andrés Codas, Kristian G. Hanssen, Bjarne Foss, Andrea Capolei, and John Bagterp Jørgensen (Computational Geosciences, 21 (2017) 479-497)</p>
CERE 1705	<p><i>“A least squares approach for efficient and reliable short-term versus long-term optimization”</i></p> <p>Lasse Hjuler Christiansen, Andrea Capolei, and John Bagterp Jørgensen (Computational Geoscience, 21 (2017) 411-426)</p>	CERE 1710	<p><i>“General approach for solving the density gradient theory in the interfacial tension calculation”</i></p> <p>Xiaodong Liang, and Michael Loch Michelsen (Fluid Phase Equilibria, 451 (2017) 79-90)</p>

CERE 1711	<p><i>“Prediction of Gas injection effect on asphaltene precipitation onset using the Cubic and Cubic-Plus-Association Equations of State”</i></p> <p>Alay Arya, Xiaodong Liang, Nicolas von Solms, and Georgios M. Kontogeorgis (Energy & Fuels, 31 (2017) 3313-3328)</p>	CERE 1716	<p><i>“Heat capacity and Joule-Thomson coefficient of selected n-alkanes at 0.1 and 10 MPa in broad temperature ranges”</i></p> <p>Teresa Regueira, Farhad Varzandeh, Erling H. Stenby, and Wei Yan (J. Chem. Thermodynamics, 111 (2017) 250-264)</p>
CERE 1713	<p><i>“Thermodynamic modeling of acid gas removal from natural gas using the Extended UNIQUAC model”</i></p> <p>Negar Sadegh, Erling H. Stenby, and Kaj Thomsen (Fluids Phase Equilibria, 442 (2017) 38-43)</p>	CERE 1717	<p><i>Freezing point determination of water-ionic liquid mixtures”</i></p> <p>Yanrong Liu, Anne S. Meyer, Yi Nie, Suojiang Zhang, Yongsheng Zhao, Philip L. Fosbøl, and Kaj Thomsen (Journal of Chemical and Engineering Data, 62 (2017) 2374-2383)</p>
CERE 1714	<p><i>“High pressure phase equilibrium of ternary and multicomponent alkane mixtures in the temperature range from (283 to 473) K”</i></p> <p>Teresa Requeira, Yiqun Liu, Ahmad A. Wibowo, Mehrshad Ashrafi, Farhad Varzandeh, Georgia Pantelide, Erling H. Stenby, and Wei Yan (Fluid Phase Equilibria, 449 (2017) 186-196)</p>	CERE 1722	<p><i>“eCPA: An ion-specific approach to parametrization”</i></p> <p>Anders Schlaikjer, Kaj Thomsen, and Georgios Kontogeorgis (Fluid Phase Equilibria (2017), https://doi.org/10.1016/j.fluid.2017.12.008)</p>
CERE 1715	<p><i>“17th International conference on petroleum phase behavior and fouling”</i></p> <p>Nicolas von Solms, Wei Yan, and Simon Andersen (Energy & Fuels, 31 (2017) 3329-3329)</p>	CERE 1725	<p><i>“An algorithm for gradient-based dynamic optimization of UV flash processes”</i></p> <p>Tobias K.S. Ritschel, Andrea Capolei, Jozsef Gaspar, and John Bagterp Jørgensen (Published online (2017)</p>



CERE 1726	<p><i>“Density and compressibility of multicomponent n-alkane mixtures up to 463 K and 140 MPa”</i></p> <p>Teresa Regueira, Maria-Lito Glykioti, Erling H. Stenby, and Wei Yan (Published online (2017))</p>
CERE 1727	<p><i>“Thermodynamic modeling of relevance to natural gas processing”</i></p> <p>Georgios M. Kontogeorgis, and Eirini Karakatsani (Chapter in the book “Natural Gas Processing from Midstream to Downstream”, Edited by Namir Elbashir, Mahmoud El-Halwagi, Ioannis Economou, and Ken Hall)</p>
CERE 1729	<p><i>“Antifreeze proteins and gas hydrate inhibition”</i></p> <p>Nicolas von Solms (Chapter in the book “Antifreeze proteins, Volume II – Biochemistry, Molecular Biology, Physical-chemistry and Applications”, Edited by Hans Ramløv and Dennis Friis, Springer Verlag)</p>
CERE 1732	<p><i>“Design and simulation of rate-based CO₂ capture processes using carbonic anhydrase (CA) applied to biogas”</i></p> <p>Philip Loldrup Fosbøl, Jozsef Gaspar, Bjartur Jacobsen, Jens Glibstrup, Arne Gladis, Kevin Milla Diaz, Kaj Thomsen, John M. Woodley, and Nicolas von Solms (Energy Procedia, 114 (2017) 1434-1443)</p>

CERE 1733	<p><i>“Pilot absorption experiments with carbonic anhydrase enhanced MDEA”</i></p> <p>Arne Gladis, Niels F. Lomholdt, Philip L. Fosbøl, John M. Woodley, and Nicolas von Solms (Energy Procedia, 114 (2017) 1158-1165)</p>
CERE 1734	<p><i>“Operating considerations of ultrafiltration in enzyme enhanced carbon capture”</i></p> <p>Maria T. Gundersen, Arne Gladis, Philip Loldrup Fosbøl, Nicolas von Solms, and John M. Woodley (Energy Procedia, 114 (2017) 735-743)</p>
CERE 1735	<p><i>“Comparison of the kinetic promoters piperazine and carbonic anhydrase for CO₂ absorption”</i></p> <p>Arne Gladis, Maria T. Gundersen, Kaj Thomsen, Philip L. Fosbøl, John M. Woodley, and Nicolas von Solms (Energy Procedia, 114 (2017) 719-725)</p>
CERE 1736	<p><i>“Rate-based modelling and validation of a pilot absorber using MDEA enhanced with carbonic anhydrase (CA)”</i></p> <p>Jozsef Gaspar, Arne Gladis, John M. Woodley, Kaj Thomsen, Nicolas von Solms, and Philip L. Fosbøl (Energy Procedia, 114 (2017) 707-718)</p>

CERE 1740	<p><i>“Solubility modeling of the systems Ni(NO₃)₂-H₂O and Fe(NO₃)₃-Ni(NO₃)₂H₂O with the extended Universal Quasichemical (UNIQUAC) model”</i></p> <p>Mouad Arrad, Mohammed Kaddami, Bahija El Goundali, and Kaj Thomsen (J. Solution Chem., 46 (2017) 1220-1229)</p>
CERE 1741	<p><i>“First study of poly(3-methylene-2-pyrrolidone) as a kinetic hydrate inhibitor”</i></p> <p>Eirin Abrahamsen, Ingrid Marie Heyns, Nicolas von Solms, Rueben Pfukwa, Bert Klumperman, and Malcolm A. Kelland (Energy & Fuels, 31 (2017) 13572-13577)</p>
CERE 1742	<p><i>“Water-oil emulsions with fines in smart water enhanced oil recovery”</i></p> <p>Muhammad Waseem Arshad, Philip L. Fosbøl, Alexander Shapiro, and Kaj Thomsen (SPE-187620-MS, (2017))</p>
CERE 1743	<p><i>“Electrical double-layer and ion bridging forces between symmetric and asymmetric charged surfaces in the presence of mono- and divalent ions”</i></p> <p>Xiaoyan Liu, Karen L. Feilberg, Wei Yan, Erling H. Stenby, and Esben Thormann (Langmuir, 33 (2017) 4426-4434)</p>

CERE 1744	<p><i>“Low field NMR surface relaxivity studies of chalk and argillaceous”</i></p> <p>Konstantina Katika, Henrik Fordsmand, and Ida L. Fabricius (Microporous and Mesoporous Materials, (2017) in press)</p>
CERE 1745	<p><i>“Low-field NMR spectrometry of chalk and argillaceous sandstones: Rock-fluid affinity assessed from T₁/T₂ ratio”</i></p> <p>Konstantina Katika, Milad Saidian, Manika Prasad, and Ida L. Fabricius (Petrophysics, 58(2) (2017) 126-140)</p>
CERE 1746	<p><i>“Complex conductivity of soils”</i></p> <p>A. Revil, A Coperey, Z. Zhao, N. Florsch, I. L. Fabricius, Y. Deng, J. R. Delsman, P. S. Pauw, M. Karaoulis, P. G. B. de Louw, E. S. van Baaren, W. Dabekaussen, A. Menkovic, and J. L. Gunnink (Water Resources Research, 53 (2017) 7121-7147)</p>
CERE 1747	<p><i>“Core flooding experiments and reactive transport modelling of seasonal heat storage in the hot deep Gassum sandstone formation”</i></p> <p>Hanne Dahl Holmslykke, Claus Kjøller, and Ida L. Fabricius (Earth and Space Chemistry, 1 (2017) 251-260)</p>



CERE 1748	<p><i>“Rock physics”</i></p> <p>Ida Lykke Fabricius (Skjæveland, S. M. and Siqveland, O. K. eds: “JCR-7 Monograph North Sea Chalk”, University of Stavanger, First Web version JCR 7 October, 2017, 39-46)</p>
CERE 1749	<p><i>“Rock properties”</i></p> <p>Ida Lykke Fabricius (Skjæveland, S. M. and Siqveland, O. K. eds: “JCR-7 Monograph North Sea Chalk”, University of Stavanger, First Web version JCR 7 October, 2017, 89-104)</p>
CERE 1750	<p><i>“Formation evaluation”</i></p> <p>I. L. Fabricius, and F. Engstrøm (Skjæveland, S. M. and Siqveland, O. K. eds: “JCR-7 Monograph North Sea Chalk”, University of Stavanger. First Web version JCR 7 October, 2017, 175-192)</p>
CERE 1751	<p><i>“Characterization and Erosion Modeling of a Nozzle-Based Inflow-Control Device”</i></p> <p>Jogvan J. Olsen, Casper S. Hemmingsen, Line Bergmann, Kenny K. Nielsen, Stefan L. Glimberg, and Jens H. Walther (SPE Drilling & Completion, Vol. 32, No. 4, (2017) SPE-186090-PA)</p>

CERE 1752	<p><i>Modeling of Shale Gas Adsorption and Its Influence on Phase Equilibrium</i></p> <p>Diego R. Sandoval, Wei Yan, Michael L. Michelsen, and Erling H. Stenby (Ind. Eng. Chem. Res., (2017) DOI: 10.1021/acs.iecr.7b04144)</p>
CERE 1753	<p><i>“Calculation of simultaneous chemical and phase equilibrium by the method of Lagrange multipliers”</i></p> <p>Christos Tsanas, Erling H. Stenby, and Wei Yan (Chemical Engineering Science, 174 (2017) 112–126)</p>
CERE 1754	<p><i>“Calculation of multiphase chemical equilibrium by the modified RAND method”</i></p> <p>Christos Tsanas, Erling H. Stenby, and Wei Yan (Industrial & Engineering Chemistry Research, 56 (2017) 11983-11995)</p>
CERE 1755	<p><i>“High pressure rheological behavior of 1-ethyl-3-methylimidazolium n-hexylsulfate and trihexyl(tetradecyl)phosphonium tris(pentafluoroethyl)trifluorophosphate”</i></p> <p>Teresa Regueira, Luis Lugo, Maria J.P. Comuñas, and Josefa Fernández J. Chem. Eng. Data, 62 (2017) 2927-2936)</p>

CERE Publications submitted in 2017

CERE 1703	<p><i>“Recycling Ionic Liquids from Water by Freeze Crystallization”</i></p> <p>Yanrong Liu, Anne S. Meyer, Yi Nie, Suojiang Zhang, Yongsheng Zhao, Philip L. Fosbøl, and Kaj Thomsen (Submitted for publication)</p>
CERE 1709	<p><i>“A massively scalable distributed multigrid framework for nonlinear marine hydrodynamics”</i></p> <p>S.L. Glimberg, A.P. Ensig-Karup, and Luke N. Olson (Submitted for publication)</p>
CERE 1712	<p><i>“Prospects of the use of nanofluids as working fluids for organic Rankine cycle power systems”</i></p> <p>Maria E. Mondejar, Jesper G. Andreasen, Maria Regidor, Stefano Riva, Georgios Kontogeorgis, Giacomo Persico, and Frederik Haglind (Accepted by Energy Procedia)</p>
CERE 1718	<p><i>“A three-dimensional model of two-phase flows in a porous medium accounting for motion of the separating surface”</i></p> <p>Alexander A. Shapiro (Submitted for publication)</p>

CERE 1720	<p><i>“Measurement of iron and lead sulfide solubility below 100°C”</i></p> <p>Diana Carolina Figueroa Murcia, Petter Lomsøy, Philip L. Fosbøl, Erling H. Stenby, and Kaj Thomsen (Submitted for publication)</p>
CERE 1721	<p><i>“Application of a crossover equation of state to describe phase equilibrium and critical properties of n-Alkanes and Methane/n-alkane mixtures”</i></p> <p>Andre P.C.M. Vinhal, Wei Yan, and Georgios M. Kontogeorgis (Submitted for publication)</p>
CERE 1723	<p><i>“The Debye-Hückel theory and its importance in modeling electrolyte solutions”</i></p> <p>Georgios M. Kontogeorgis, Bjørn Maribo-Mogensen, and Kaj Thomsen (Submitted for publication)</p>
CERE 1724	<p><i>“A fast and memory-efficient spectral galerkin scheme for distributed elliptic optimal control problems”</i></p> <p>Lasse H. Christiansen, and John B. Jørgensen (Submitted for publication)</p>



CERE 1737	<i>“A least squares method for ensemble-based multi-objective oil production optimization”</i>
	Lasse Hjuler Christiansen, Steen Hørsholt, and John Bagterp Jørgensen (Submitted for 3rd IFAC Workshop on Automatic Control in Offshore Oil and Gas Production)

CERE 1738	<i>“Production optimization of a rigorous thermal and compositional reservoir flow model”</i>
	Tobias K.S. Ritschel, and John Bagterp Jørgensen (Submitted for 3rd IFAC Workshop on Automatic Control in Offshore Oil and Gas Production)

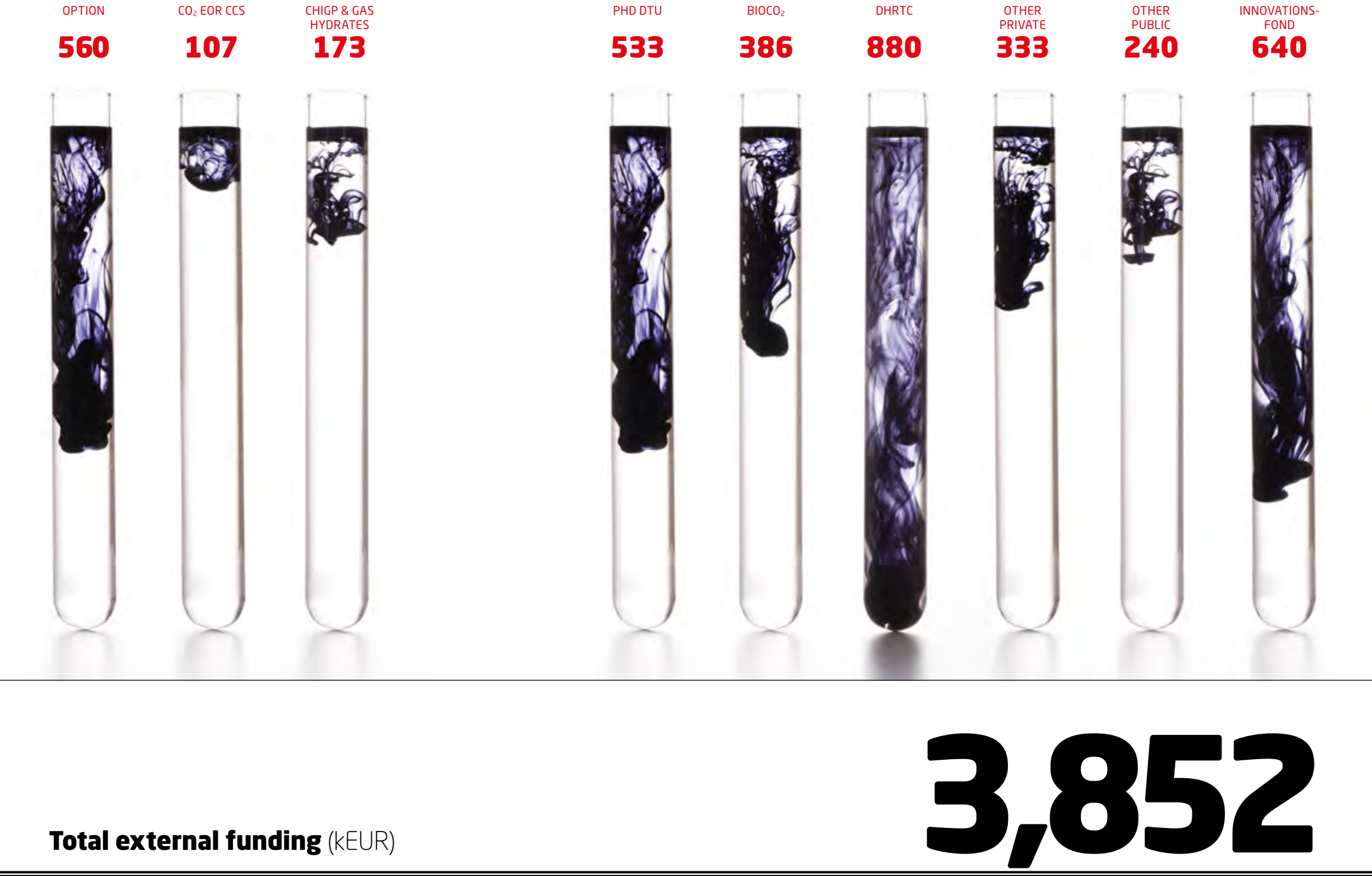
CERE 1739	<i>“Oil production optimization of black-oil models by integration of Matlab and Eclipse E300”</i>
	S. Hørsholt, H.M. Nick, and J.B. Jørgensen (Submitted for 3rd IFAC Workshop on Automatic Control in Offshore Oil and Gas Production)

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):



Staff 2017

Faculty



Ida Lykke Fabricius
DTU Civil Engineering



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