Technical University
of Denmark

CERE ANNUAL REPORT 2016

Electronic Version of the CERE Annual Report 2016

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

Publications in 2016
CERE performs well in the world of energy resources engineering. This is reflected in the publications produced every year. The full list of 2016 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 2016 Master's Theses is found in the e-report.

CENTER FOR ENERGY
RESOURCES ENGINEERING

CERE Annual Report 2016

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Chalk cores with varying degrees of oil saturation.

Diversity and Flexibility is our Strength

Professor
Georgios
Kontogeorgis,
Chairman of CERE
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Welcome to the 2016 CERE Annual Report! 2016 was a challenging year both for us in CERE and for several of our member companies due to modest oil prices and other reasons. Challenging years call for new solutions, new collaborations and new directions, while building further on our own expertise. The expertise of the center's faculties within e.g. applied thermodynamics, mathematical modeling, process simulation, geology and geophysics can be used in a variety of applications. Indeed this diversity and flexibility constitute strengths of CERE.

Two highly interdisciplinary projects, NextOil and HeHo, approach the conclusion of their planned durations. The former is focused on deep oil exploration – also known as HPHT (High Pressure, High Temperature) – while the latter investigates geothermal energy resources. Both projects have generated impressive results within modeling and experiments. We are confident that the advanced experimental facilities built in NextOil and the solid expertise on geothermal energy generated in HeHo will find use in future research projects.

Highlights from a busy year

Thermodynamics is one of the main research areas of CERE and three PhD projects started this year, one experimental on multicomponent multiphase measurements for complex systems and two modeling ones on advanced theories for interfacial tensions and modeling of complex hydrate promoters for CO_2 capture. These three projects will tackle complex modeling and experimental aspects of applied thermodynamics. In all three projects we expect that advanced thermodynamic models like CPA and SAFT will be used. Advances in thermodynamics often yield new software. We expect significant new developments and further organization and presentation of software for the member companies during 2017.

A major event in 2016 was the Petrophase conference in June, shortly after the CERE Discussion Meeting. CERE faculties Nicolas von Solms and Wei Yan were the chairmen of the conference. This was the second time the conference was held in Denmark and with 150 contributions from 180 attendees (including 5 invited speakers and 40 plenary talks) we note this as a great success.

Several research activities at CERE within enhanced oil recovery and other upstream oil topics are based on funding from and collaboration with the Danish Hydrocarbon Research and Technology Center (DHRTC). CERE faculties gave invited lectures at the DHRTC conference in November, and DHRTC researchers attended the CERE discussion meeting in June. Further, some of our technical personnel are involved in DHRTC projects. In other words, there is strong synergy between CERE and DHRTC. We expect that this trend will not just continue but even intensify in the years to come.

New frontiers opening up

Last year, a major project coordinated by CERE within bio-energy was initiated. The SYNFERON (optimized SYNgas FERmentatiON for biofuels productions) is now at full speed. The project is funded by Innovation Fund Denmark and involves collaboration with several companies and three other research groups from DTU Chemical Engineering. It is a truly interdisciplinary project, where CERE expertise in process simulation is used, besides the coordination responsibility.

Several new CERE projects were granted during 2016

The aim of the BIOCO2 project is to develop and test a new efficient way of upgrading biogas for the combined production of bio-methane and high-quality CO_2 ($bioCO_2$). The project involves collaboration between CERE, DTU, Union Engineering A/S, and Danish Gas Technology Centre and has a total budget of 14 million DKK (1.9 million EUR). The project has received funding from the Danish Energy Agency's Energy Technology Development and Demonstration Program (EUDP). Associate Professor Philip L. Fosbøl, CERE, is Principal Investigator.

CERE Professor Ida Fabricius is part of a consortium consisting of CERE, DTU, three industrial companies, and The Geological Survey of Denmark and Greenland (GEUS) who has received a grant from the Danish EUDP foundation for a research project on geothermal energy storage.

Finally, Senior Researcher Arne Døssing, member of the CERE faculty, has received funding for a new project on drones for high-quality magnetic surveying with relevance to applications such as discovery of mineral or energy resources such as oil and gas, as well as geothermal reservoirs. External project partners are Sky-Watch, Geo, DONG Energy, and Royal Danish Navy EOD Service. Funding is provided mainly by Innovation Fund Denmark. The project has a total budget of 16 million DKK (2.2 million EUR).

Looking ahead

2017 will include several new initiatives. I have already mentioned a clearer presentation of the software at the CERE members' website with more software tools being available for the consortium.

We celebrated five PhD defenses from CERE students during 2016, all of which were distributed to the CERE consortium, just as they are available at the CERE members' website. We are also happy to see so many of our previous PhD students and postdoctoral researchers keeping in touch and visiting the center. We have therefore decided to establish a CERE Alumni initiative consisting of all previous PhD and postdocs from CERE (and previously IVC-SEP) as we expect many of them may be interested in following the center's activities.

Besides CERE's Discussion Meeting, no other conferences are planned for 2017, thus taking a break from two consecutive years in organizing international conferences. I wish to express my own and the center's gratitude to our industrial consortium for the continuing support in all ways, including extensive communication in existing and recently funded projects, as well as for being interested in participating in future research applications.

On a final note, we expect that 2017 will be an exciting year in many respects. While continuously building on our expertise, certain new broader collaborations may take place.

I hope you will find the annual report useful and informative. Any comments and suggestions from the CERE consortium members and other stakeholders are, as always, most welcome.

I hope to see you at the annual CERE Discussion Meeting 2017 in June!

Professor Georgios Kontogeorgis,
Chairman of CERE

Voices of the CERE Industrial Consortium

CERE strives for active cooperation with the members of its industry Consortium. But how do representatives of the companies view things?

Technical expert Birol Dindoruk, Shell International, USA:
"If you look at the many projects in CERE, they are like Lego bricks. They each have value, but if you combine them, they fit and form a larger structure. What I find especially interesting is the fact, that companies trust CERE with actual production data. This is quite rare for an academic institution, and it increases the value for us, since the proposed solutions will be closer to realization."

Birol Dindoruk is Principal Technical Expert of Reservoir Engineering, and one of only eight principal technical experts in Shell International. He works in Projects & Technology, formerly known as Shell Technology Center Houston. Asked whether CERE is able to strike an acceptable balance between academic and practical interest, he replies:

"It can never be too academic! CERE's work should be academic. To my experience, you can always find an application. And if I come here and find just one thing, which is really useful, well, mission accomplished."

Still, while the work itself should be academic, it is also important to have an eye for dissemination, he stresses:

"First of all, we are always interested in access to software code. We want to be able to test the solutions developed by academia in-house. And we appreciate the efforts that CERE puts into making their software available in SPECS and other formats. Also, exchanging people – like summer students – is a good way to disseminate results."

Last, but not least the ongoing contact is important to Birol Dindoruk:

"When I send an email to a member of the CERE faculty, I know they will attend to my question and come back with a useful answer. In my domain everybody knows this place – even though Denmark is not that known for oil and gas activity. This is mainly due to people. The faculty of CERE is a good group, and something Denmark has reason to be proud of."

PhD Michele Mattei, AkzoNobel, The Netherlands:
"Since AkzoNobel joined the Consortium in 2002, the tendency has been for CERE to lean towards oil and gas, but the activities are still highly relevant for the specialty chemicals industry. A number of the issues we have in process design and

AkzoNobel Research, The Netherlands
BP Chemicals Limited, United Kingdom
Calsep, Denmark
Chevron, USA
ConocoPhillips, USA
DONG Energy, Denmark
ExxonMobil Research and Engineering, USA
Gassco AS, Norway
Gassnova SF, Norway
GDF SUEZ, France
Haldor Topsøe A/S, Denmark
Hess Danmark ApS, Denmark
IFP Nouvelles Energie, France
KBC, United Kingdom
Linde AG, Germany
Lloyd's Register Consulting, Denmark
Maersk Oil, Denmark
MOL Group, Hungary
National Oilwell Varco Denmark I/S, Denmark
OMV E&P, Austria
Petrobras S.A., Brazil
RWE Dea, AG, Germany
Schlumberger, USA
Shell Global Solutions International B.V., The Netherlands
SINOPEC, P.R. China
SQM SA., Chile
Statoil, Norway
TOTAL, France
Union Engineering, Denmark
Welltec, Denmark

Voices of the Industry Consortium
More than 30 highly international companies play active parts in the activities of CERE. From the left: Birol Dindoruk, Shell International; CFD Specialist Line Bergmann, Welltec; Physicist Xiaohong Zhang, KBC Advanced Technologies Ltd; Researcher Michele Mattei, AkzoNobel

control are very similar to the oil and gas industry, and the same solutions can often be applied."

As a leading producer of paint and coatings, and a major producer of a range of specialty chemicals, AkzoNobel supplies essential ingredients, essential protection and essential color to industries and consumers worldwide. The company has more than 45,000 employees in more than 80 countries. There are 4,000 scientists and technologists; Michele Mattei is in specialty chemicals research.

"This is the field closest to the activities of CERE."

As an example, Michele Mattei points to electrolyte thermodynamics. CERE has developed new models and software in this field which is highly relevant to AkzoNobel, as the company is the world leader in refined salt.

"One thing I like a lot in CERE's efforts is the balance between modeling and experiments. You need to constantly link both types of developments. When experiments and model predictions differ we tend to always blame the model. This is really not fair. Both experiments and models contribute to uncertainty. You need to always keep the full picture in mind. Rather that striving for a model that is fully predictive, thus not requiring any experiment, from an industrial perspective it is more productive to use semi-predictive approaches, where few dedicated experiments can be used to extrapolate results to a wider range. Combining experiments and modeling results with uncertainty indications, however, is in general gaining interest in industry, and my recommendation to CERE would be to also pay attention to this development."

Physicist Xiaohong Zhang, KBC Advanced Technologies Ltd, UK.
"One of the key KBC software products is Petro-SIM, a process simulator powered by the well-established thermal engine, Multiflash. In order to keep improving our software technology, we are always keen in seeking new ideas and methods."

KBC, recently acquired by Japanese Yokogawa Electric Corporation, provides software solutions and technical consultancy to the global oil and gas, petrochemical and gas processing industry. Xiaohong Zhang is a senior technical developer at KBC. She has worked for nearly 20 years in chemical engineering, particularly in the development of thermodynamic models for modelling the phase behavior of gas hydrates, waxes and asphaltenes. She has been following the work of CERE for a number of years. In 2016 she attended her first CERE Discussion Meeting.

"The Discussion Meeting is an inspiring place to go, and is an excellent forum to follow any new developments in the relevant disciplines," says Xiaohong Zhang, "It is also a place where we can meet not only the students at CERE but also the people from oil and gas industries. The Master and PhD students at CERE have a good attitude to the research work. Their curiosity, determination, hard work and excellent input from the DTU staff are the keys to their success in producing high quality results. The industries surely benefit from the projects carried out by the students at CERE".

CFD Specialist Line Bergmann, Welltec, Denmark:
"We were attracted by the scope of the OPTION project, which is to ensure that results will not only be of academic interest, but will be applicable to industry. We already provide our clients with hardware in terms of valves and packers for zonal isolation and stimulation, production, and injection. We sincerely believe that the software solutions developed in the OPTION project can be combined with the Welltec completion to provide even stronger solutions."

Line Bergman is Computational Fluid Dynamics (CFD) Specialist at Welltec. The company provides well technology for the oil and gas industry. This includes both well completion technology and intervention solutions. Welltec is strongly engaged in the CERE led Joint Industry Project OPTION (Optimizing Oil Production by Novel Technology Integration).

"To take the completions as an example, we face a number of challenges related to scaling, corrosion etc. Which materials should we choose, and which coatings? These questions are all addressed in various CERE projects. And obviously, a wide range of software solutions have our interest. Finally, it is very inspirational to hear experiences from other companies."

In OPTION, Line Bergmann heads the work package on near-well flow simulations. Usually, the work packages in CERE's joint industry projects are headed by CERE faculty members.

"Coordinating the work package does consume a fair amount of my time, but we have found a fine routine. The two DTU students involved spend a weekly day at Welltec, and also a day at Lloyds Register. This is a smooth way of securing ongoing progress and coordination."

The CERE Discussion Meeting

The four interviews took place at the CERE Discussion Meeting 2016. As always, this annual event attracted a large number of both industrial and academic participants – totaling 95, of which no less than 24 represented companies in the Industry Consortium, while five participants were from other companies. Most industry representatives were from the oil & gas sector, but also four companies from other industry sectors were also present. The meeting was held at the Marienborg Hotel, Helsingør, on June 13-15.

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.

A Danish Potential for deep Heat Storage

A clear Potential for Geothermal Energy. Heat can be injected into Danish sandstone aquifers during summer and retrieved during winter.

Research coordinated by CERE shows that hot water can be injected into deep Danish sandstone aquifers during the summertime, and heat be retrieved during the winter.

Several Danish towns and cities can have their heating supply covered by a combination of heat storage in deep aquifers and geothermal energy. This conclusion is based on a five-year research program at CERE, HeHo (Heat Storage in Hot Aquifers).

According to simulations in the project, it is possible to inject hot water into certain deep sandstone aquifers in Denmark and retrieve 50 % of the heat after six months. This figure may not sound too impressive, but is actually enough for the solution to be highly relevant.

"During the summertime, the demand for heating is obviously very low, and you have a large surplus of heat energy which is more or less wasted today. Storing this energy in the ground instead, and retrieving it during the winter when the demand is high, would introduce a cheap and carbon neutral resource – even if half of the energy is lost," says Professor Ida L. Fabricius, coordinator of HeHo.

"Further, the economic feasibility of the solution can be improved by combining the energy storage with geo-thermal production. Once you have the infrastructure for geo-thermal energy production in place, it will be relatively cheap to add deep energy storage."

The first model for the purpose

A major source of summertime surplus heat is water heated by the sun in solar farms. Further, a number of countries including Denmark are extending their production of bio-energy. It might be economically rational to let these plants run throughout the year and let the heat produced in the summertime be stored for later use. The same thing applies to incineration of waste which is also used for heating purposes. The systems require for the waste to be burned throughout the year. Presently part of the heat is just being wasted in the summertime.

"The concept would be especially interesting for a country like Denmark where district heating is already advanced. One could use the geothermal and stored heat directly for district heating," Ida L. Fabricius emphasizes.

The HeHo research team has gone to great lengths to verify the accuracy of their simulations. A key parameter in heat conductivity estimates is the distribution of clay in the sedimentary rock layers. The geology team at CERE presented these basic data in a state-of-the-art commercial software for the purpose, Schlumberger's "Petrel". The data were then processed further by Professor Klaus Mosegaard of University of Copenhagen (CERE associated faculty) into a mathematical model yielding a number of possible clay distributions.

"Joining different scientific disciplines in this manner is a trade mark for CERE. As a result we are the first group to have developed a model for heat conductivity in sedimentary rock structures. It was always our belief that you need to be able to include accurate parameters for the specific geological structure for the results to be of value," says Ida L. Fabricius.

Integration of local geology is imperative

The group has an ongoing collaboration with a group at the Korean Advanced Institute of Science and Technology (KAIST). This group, led by Professor Seung Rae Lee, specializes in heat conductivity simulations, but in a quite different type of geology at much lower depth.

"Initial simulations by the KAIST group suggested that we would be able to retrieve as much as 70 % of the injected heat. However, this was based on an assumption of a homogeneous geology. We remained skeptical, and insisted on creating a model with a more accurate geological description, as the geology of the Danish aquifers in question is rather diverse. This correction has lowered the estimate from 70 % heat retrieved to 50 %," Ida L. Fabricius explains.

"A difference of this magnitude is obviously significant to a municipality or an energy corporation considering an investment. Thus we are pleased that we took the effort to integrate the actual geology accurately."

Gassum sandstone is ideal

The HeHo project has addressed two distinct geological structures, namely Danish Gassum Formation sandstone and Bunter Formation sandstone respectively. Both are found at depths around 1.5-2.0 km in Denmark. This is an attractive depth as the temperature is quite high, implying a lower heat gradient and thus a smaller loss of heat when hot water is stored.

Although the heat gradient is lower at these depths, there is a risk of deterioration of the reservoir quality when hot water with increased temperature is introduced in the sandstone reservoirs. Therefore, as a part of the project a series of high quality geochemical experiments at in situ pressures and temperatures were led by Head of Laboratory Claus Kjøller at the GEUS Core Laboratory.

"Our laboratory experiments with Bunter sandstone at GEUS were unfavorable. When Bunter sandstone is exposed to hot water injection over prolonged intervals, it tends to crumble. Fortunately, the same was not seen in Gassum sandstone which has a higher content of pure quartz grains. We would therefore recommend that future exploitation of this type of energy storage takes place in Gassum sandstone," the HeHo coordinator states.

A further recommendation is to choose, if possible, Gassum sandstone with a relatively low content of the mineral kaolinite, which tends to plug sandstones pores and thereby reduce permeability.

Ready once energy policy changes

As Gassum sandstone is found widely in the Danish geology, the potential for heat storage in deep aquifers in Denmark is clear. Still, it has been beyond the scope of the work in HeHo to provide an overall estimate of the total national potential.

"This would require a more detailed mapping of the geology. Further, the pattern of consumption is also relevant – it would be preferable to use the method in locations with a matching demand for heating," says Ida L. Fabricius, noting that policy developments since the start of the HeHo project five years ago have not been favorable:

"Unfortunately, the present energy policy and the current regime of energy prices and subsidies do not favor heat storage in deep aquifers. Still, the project has been a success from a scientific point of view. We now have a model in place which can be put to use instantly, once the energy policy environment changes back in favor of geo-energy."

Forward this article

Ida L. Fabricius, professor

Lisa Pasquinelli, PhD student

Tobias Orlander, PhD student

The HeHo project

The Heat Storage in Hot Aquifers project (HeHo), is a research collaboration including DTU, GEUS, the University of Copenhagen, and the Danish District Heating Association. Funding was provided by the Danish Council for Strategic Research. The project ran from 2011 to 2016.

Sub-surface Heat Storage for Copenhagen

A consortium with CERE participation has received funding for a project on thermal heat storage in subsurface limestones of the Copenhagen area.

Underground storage of energy will become an important part of the Danish energy system, as it may contribute to the necessary leveling out of large variations in energy production and consumption. Also, it may contribute to exploit surplus heat from industry, waste incineration and power production.

The project, entitled High Temperature Energy Storage (HTES), aims to demonstrate thermal storage in subsurface limestones, integration into a practical context in the district heating sector, and gaining operational experiences with the technology for subsequent commercialization.

The heat supply for the HTES system will originate from surplus production from combined heat and power units, industrial surplus heat, and surplus heat from sun farms.

The HTES consortium consists of CERE, the Geological Survey of Denmark and Greenland (GEUS), and three industrial companies – Ross DK (Coordinator), GEO, and OE3i.

The project is made possible by a grant from the Danish Energy Agency's Energy Technology Development and Demonstration Program (EUDP). The HTES project has a total budget of 740,000 EUR. The project will run from 2017 to 2020. One PhD student will employed at CERE.

Henrik Lund Nielsen investigating ship engine corrosion electrochemically with a Rotating Disk Electrode setup.

Addressing a tricky Corrosion Problem in Ships

To save fuel, cargo vessels often operate at reduced loads. Unexpectedly, this has led to sulfur-caused corrosion problems in engines. CERE takes part in an effort that will help ship owners achieve the desired savings without corrosion.

To save fuel, cargo vessels often operate at reduced loads. Unexpectedly, this has led to sulfur-caused corrosion problems in engines. CERE takes part in an effort that will help ship owners achieve the desired savings without corrosion.

When a cargo ship saves fuel, economic feasibility is increased, and both climate change impact and exhaust of environmentally harmful substances are reduced. This has led ship owners across the world to take an interest in "slow steaming". I.e., when the schedule of a cargo ship allows it, velocity will be reduced in order to optimize fuel consumption relative to distance. But in some cases, the achieved savings are endangered, as the changed conditions of operation trigger corrosion in the engines.

"When these problems were first seen, it was quite surprising. One would not expect that lowering the temperature inside the engine from about 200 °C to about 150 °C would increase corrosion, as in both cases water would evaporate completely. However, it seems that a temperature of about 150 °C allows for tiny droplets of water to persist for just long enough to create problems – something which was never seen when the temperature of operation was around 200 °C," explains Associate Professor Philip L. Fosbøl, CERE.

CERE takes part in the SULCOR project – an effort led by DTU Mechanical Engineering, and with engine manufacturer MAN Diesel & Turbo as the main industrial partner. Besides CERE, another group at DTU Chemical Engineering, CHEC, is involved.

A hostile, corrosive environment

The name SULCOR refers to the realization that sulfur-containing substances are the main cause of the corrosion problems during slow steaming. Sulfur oxides formed during combustion in diesel engines can oxidize to SO_3 and, in the presence of water, form sulfuric acid, which acts as the corrosive agent. Commercial alkaline lubrication oil, containing surfactants and limestone, acts to neutralize the acid, but presently offers insufficient protection.

The de-facto standard propulsion technology for large commercial cargo vessels is the marine low speed two-stroke Diesel engine. The cylinder of a ship engine is a hostile environment in relation to corrosion protection, with a strongly turbulent and transient gas-phase at high pressure and temperature interacting with an oil emulsion of 1-5 µm thickness. This physical and chemical complexity makes an understanding of the rate-limiting phenomena in the corrosion process challenging.

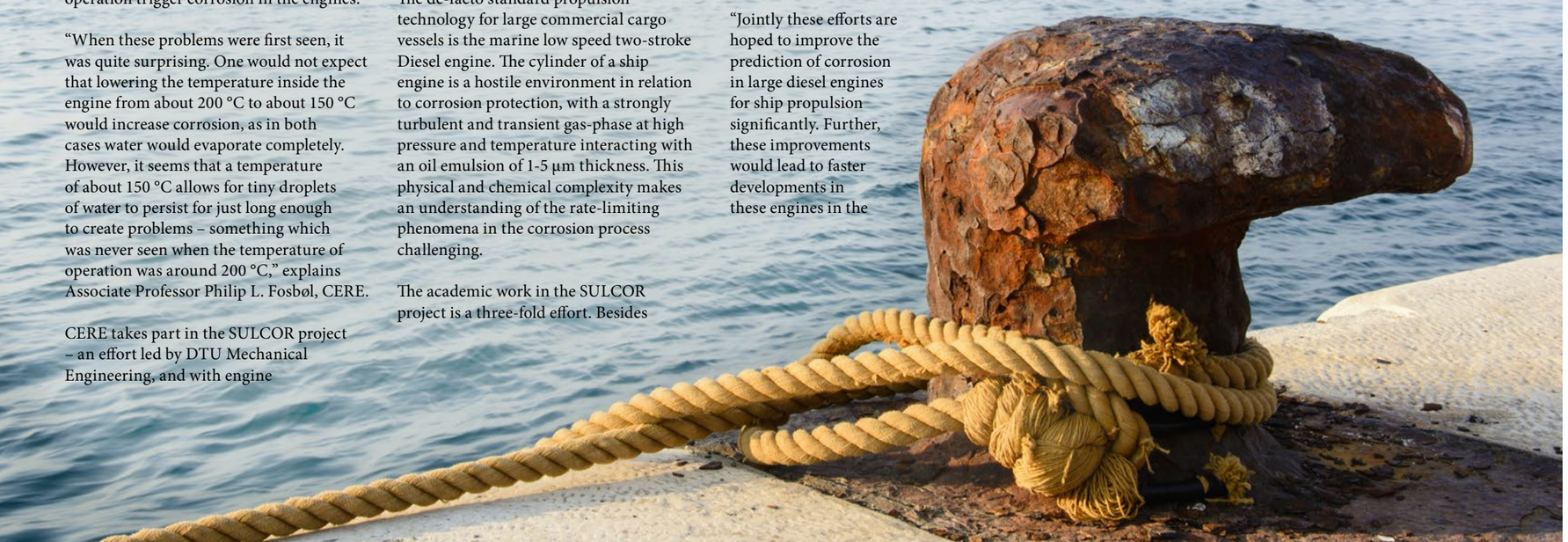
The academic work in the SULCOR project is a three-fold effort. Besides overall coordination, the group at DTU Mechanical Engineering undertakes materials science and practical engine tests, while the CHEC-group at DTU Chemical Engineering investigates interactions between sulfuric compounds and the lubrication oil. And finally, CERE investigates the involved mechanisms of corrosion.

Broader relevance to combustion

The model tools in the project will include a multi-zone model that calculates the amount of sulfuric acid condensing on the cylinder liner, a heat and mass transfer model for the turbulent boundary layer near the wall, and a model for the physical/chemical neutralization of sulfuric acid in the lubricant film on the cylinder liner.

"Jointly these efforts are hoped to improve the prediction of corrosion in large diesel engines for ship propulsion significantly. Further, these improvements would lead to faster developments in these engines in the efforts to meet stricter regulations on fuels, fuel consumption, and emissions," says Philip L. Fosbøl, noting that the shipping industry faces increasing demands to cut emissions of sulfur oxides (SOx), nitrogen oxides (SOx) and carbon dioxide (CO_2).

"The work in SULCOR is directly relevant to sulfur corrosion issues in large marine engines resulting from "slow steaming". However, the mechanisms that are developed in the mathematical tools will have an impact on the modelling of many other combustion applications as well," Philip L. Fosbøl concludes.



Henrik Lund Nielsen, PhD student

Philip L. Fosbøl, Associate Professor

Forward this article

The SULCOR project

Over 90 % of the world trade is carried by the international shipping industry. In the next 5-10 years stricter regulations on pollution from cargo vessels are coming into force. The main driver in this field is demands set by the International Maritime Organization (IMO) on new-built ships. Also, some individual countries and local authorities choose to put environmental demands on ships. For instance, ships with high emissions of nitrogen oxides – associated with a number of health issues – face restrictions in terms of which harbors they are able to access.

At the same time more stringent regulations on the sulfur content of fuels are introduced. As a consequence, both the design of ship engines and operation will need to be changed. One of the major challenges will then be to prevent "cold corrosion" in the engines. Here "cold" is a relative term – meaning a lower temperature than the approx. 200 °C which used to be the standard operating temperature. Cold corrosion is a mixture of acid attack and mechanical wear in the engine, caused by sulfuric acid condensing on the cylinder walls to a greater extent than at higher temperatures.

DTU and engine manufacturing corporation MAN Diesel & Turbo have teamed up in the SULCOR project in order to understand and avoid these corrosion problems. The project involves leading international experts. Financing is provided by Innovation Fund Denmark. The project is coordinated by DTU Mechanical Engineering and will end by early 2019. At CERE, Henrik Lund Nielsen is employed as a PhD student in the project.

Carolina Figueroa at work with the HPHT titanium cell in CERE's lab.

Scaling during deep Oil Exploration

While scaling problems may not overall be larger during High Pressure, High Temperature (HPHT) oil and gas exploration compared to conventional exploration, the challenges certainly are different. CERE is committed to provide a basis for predicting the "exotic" scaling during HPHT.

Through a combination of experiments and modeling, CERE has made significant progress in providing much needed predictions of the levels of scaling which can be expected during High Pressure, High Temperature (HPTH) oil and gas exploration.

"To someone outside the energy resources sector, scaling may seem to be a rather small issue compared with the many other technology challenges involved in deep exploration. However, if you don't pay attention to it, scaling can be really costly to a company. Industry is fully aware of this fact," says Carolina Figueroa, PhD-student at CERE.

With dwindling easily accessible oil and gas resources, interest in deeper reservoirs is rising. Deeper reservoirs mean higher temperatures and pressures. Reservoirs above 150 °C and 700 bars are classified as high pressure high temperature (HPHT) reservoirs. Many of these reservoirs are found offshore, including the North Sea.

Deep exploration triggers "exotic" scaling

Deposition of minerals, or scaling, is a challenge in any kind of oil and gas exploration and production. While the formation water in a reservoir will be in equilibrium with the rock, this changes as production is commenced. Then, ions present in the formation water in solution will begin to precipitate. Under certain conditions the deposited minerals can form a layer on the inner walls of pipes and other equipment. Over time this layer can grow to a thickness causing production losses and even total stop of production, also known as "clogging".

In conventional oil and gas exploration, the most common scaling materials are carbonates and sulfates of barium, strontium, calcium and magnesium. Under the extreme conditions in HPHT, several other scaling materials are seen.

"Compared to the more common scale materials, these "exotic" scale materials are characterized by extremely low solubility. While this is bad news in the sense that the scaling materials will precipitate easily, it is good news in the sense that the amounts will be lower compared to the most common types of scaling," Carolina Figueroa explains.

Also, such additional scale materials are bad news later in the production process. I.e. refineries will have techniques in place to handle the well-known scale materials in oil, but not the ones seen only in oil from HPHT.

Know your scaling in advance

Various techniques do exist to remove scales, but they all involve certain challenges.

"If you use chemistry, you will introduce new substances to the oil and thereby have certain issues at the later stages including at the refineries. And even if you limit yourself to mechanical techniques, you risk similar problems, because the scraping of the inner pipe walls will typically increase corrosion problems, which again may induce the formation of e.g. iron sulfide (FeS). Further, it will be both more difficult and more expensive to remove scales at large depths compared to conventional exploration. So all in all, preventing the scaling in the first place will be highly desirable," says Carolina Figueroa.

Examples of scale materials especially associated with HPHT are zinc sulfide (ZnS), lead sulfide (PbS), and iron sulfide (FeS).

"Of these, the iron source for FeS is not naturally occurring in the reservoirs, but stems from corrosion in the production equipment. Thus, iron sulfide scaling can actually be limited by better corrosion control. For zinc sulfide and lead sulfide it will be much harder to prevent occurrence. But at least one can predict at which levels and which depths this scaling will take place, in order to manage the challenge better. Further, knowing the magnitude of these challenges will enable a company to include cost estimates in its economic feasibility studies prior to exploration rather than being caught by surprise," says Carolina Figueroa.

No "rule of thumb" to adhere to

The team has initially focused on zinc sulfide (ZnS). Through both experiments and modeling, ZnS is now included in the group of scale materials which can be modelled with the Extended UNIQUAC model.

Prediction of ZnS scaling requires an elaborate effort, Carolina Figueroa explains:

"Unfortunately, there is no "rule of thumb" to adhere by such as scaling increasing or decreasing with increasing temperature and pressure. Rather, the scaling takes place at certain specific conditions over certain temperature and pressure intervals. Moreover, a company considering a HPHT project cannot just focus on the conditions at the given reservoir depth but will need to take all conditions from the surface to the reservoir depth into account."

This situation has also been challenging for the CERE team.

"We are confident that the Extended UNIQUAC model is a useful model for the purpose. However extensive experimental work covering a wide range of temperatures and pressures is absolutely necessary to verify and potentially adjust the model."

Titanium cell copes with high pressure

Experiments up to 200 °C and 60 bars are being conducted at a HPHT titanium cell. This cell has been designed and built at CERE for HPHT solubility analysis purposes. While a temperature of 200 °C is realistic, the pressure under actual exploration will go much higher than 60 bars.

"We settled for 60 bars as the Extended UNIQUAC model includes parameters to represent the solid-liquid equilibrium at further pressures. 60 bars is a fairly high pressure, and as the experimental results and the model predictions are in agreement, we are confident that the model will accurately predict scaling at higher pressures," says Carolina Figueroa.

In other words, the team has shown the Extended UNIQUAC model to be capable of predicting ZnS scaling in HPHT reservoirs. The methodology can be extended to other scaling materials such as PbS and FeS, making the model a leading tool for prediction of scaling in HPHT reservoirs.

Besides including other exotic scale materials than ZnS, the team sees several other future developments:

"Presently, we have only addressed the water and ZnS system, but in real exploration you will see interactions with other ions as well. More work is needed to include such interactions, and also to describe the kinetics involved."

Carolina Figueroa, PhD student

Kaj Thomsen, Associate Professor

Philip L. Fosbøl, Associate Professor

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NextOil

The effort on HPHT scaling is a part of the Next Oil project (New Extreme Oil and Gas in Denmark) led by CERE. The project is sponsored by Innovation Fund Denmark, DONG Energy, and Maersk Oil. It was initiated in 2012 and is due to end by the summer of 2017. The project involves work packages on scaling, on rock mechanics and on hydrocarbon reservoir fluids. Besides Carolina Figueroa (interviewed) PhD students are Farhad Varzandeh and Tobias Orlander, while Teresa Regueira is Postdoc. Professor Erling H. Stenby, DTU Chemistry, is the Principal Investigator of Next Oil.

20 Years with the CPA Model

Several CERE projects evolve around the Cubic Plus Association (CPA) thermodynamic model, which allows for the description of complex mixtures relevant to contemporary energy resources engineering. An example could be water and hydrocarbons with methanol or glycols. The article gives a status for the CPA – and looks ahead.

Contemporary energy resources engineering is complex. Often hydrocarbons are mixed with gases like CO_2 and H_2S, water and other polar chemicals, e.g. methanol and glycols. These chemicals are used as gas hydrate inhibitors and are important during the processing and transportation of oil and gas. Sustainable and economically feasible production and transportation of oil requires careful control of these chemicals both in terms of type and amount used.

A key factor in these efforts is knowledge of thermodynamics. For example, the thermodynamics is directly related to the necessary amount of inhibitors injected for specific applications and the knowledge of the chemicals' fate in the ecosystems, especially aquatic ones. Accurate knowledge of phase behavior and other thermodynamic properties of these mixtures is necessary in optimizing the amount and nature of chemicals used in the downstream oil industry.

CPA (Cubic-Plus-Association) is a thermodynamic model first published in 1996, as part of a collaboration with Shell and Infochem (now KBC), both members of the CERE Industry Consortium. The model combines the cubic equation of state – used as standard in the oil and gas industry - with an explicit association term which accounts for complex interactions when polar chemicals like water, methanol and glycols are present. The association term was developed a few years earlier in the context of the SAFT model, but was never really used until the advent of CPA.

Today, the CPA is widely accepted as a successful model in the oil and chemical industries, as well as for applications related to CO_2 capture and storage. Since 1999, a joint industry project at CERE (CHIGP) has ensured the further development and industrial application of CPA. Several member companies have participated in CHIGP, with Statoil, BP and Petrobras being the current members.

Wide use in academia and industry

The main merit of the CPA is its ability to predict phase equilibria and other thermodynamic properties of hydrocarbons, gases, water and other polar chemicals. Using adjustable parameters solely obtained from binary systems, CPA can predict phase behavior for mixtures containing any type of hydrocarbons, gases, water and a variety of polar chemicals (e.g. water, glycols, acids, amines and alkanolamines). This assists the oil industry in a number of fields, including environmental applications e.g. optimizing the use of chemicals and CO_2 capture and storage. The predictive capability is the strength of the model, as rather few experimental data are available for multicomponent systems encountered in most industrial applications.

Keen CPA users can be found both in academia and in industry.

The impact on the academic side can be seen by the fact that over 30 research groups in universities in Europe, USA, Africa and Asia have used CPA extensively and further extended the model to more applications, e.g. mixtures containing biodiesel, pharma-

ceuticals, complex multifunctional molecules, asphaltenes, critical phenomena, solubility parameter estimation, electrolytes, and polar compounds. A book authored by Dr. G. Folas and CERE Chairman G. Kontogeorgis in 2010 on association models including CPA and SAFT currently has over 350 citations.

On the industrial side, many companies are actively using CPA, which has been extensively applied to CCS applications, reservoir fluids and electrolytes. Finally, ASPEN (the world's largest simulation company) has recently included CPA in their simulator, AspenPlus.

Large save in methanol consumption

The results are published in the open literature and the CPA model is not patented. The model is disseminated to industrial and other interested parties in the form of software suitable for use in process simulators (CAPE-OPEN compliant and AspenPlus user model). There are also other providers of the CPA model, and several CERE member companies have their own implementations of CPA. Successful industrial applications include gas hydrate inhibition, reservoir fluid phase behavior, water content of gas, chemicals, etc. One company reported that the accuracy of the CPA model has enabled them to reduce their use of methanol as hydrate inhibitor by 40 %. This is a good illustration of the potential cost benefits of more accurate physical property models; it is also environmentally beneficial if excess use of chemicals can be reduced.

The focus during recent years has been demanding applications like electrolytes, asphaltenes, critical region and interfacial phenomena (including both surface tensions and multicomponent adsorption), measurements (in-house multicomponent vapor-liquid-liquid equilibria and in collaboration with Statoil for reservoir fluids) as well as extensive dissemination efforts including enhancing existing software implementations (CAPE-OPEN, AspenPlus user model) and developing new ones using MATLAB for the electrolytes and asphaltene developments.

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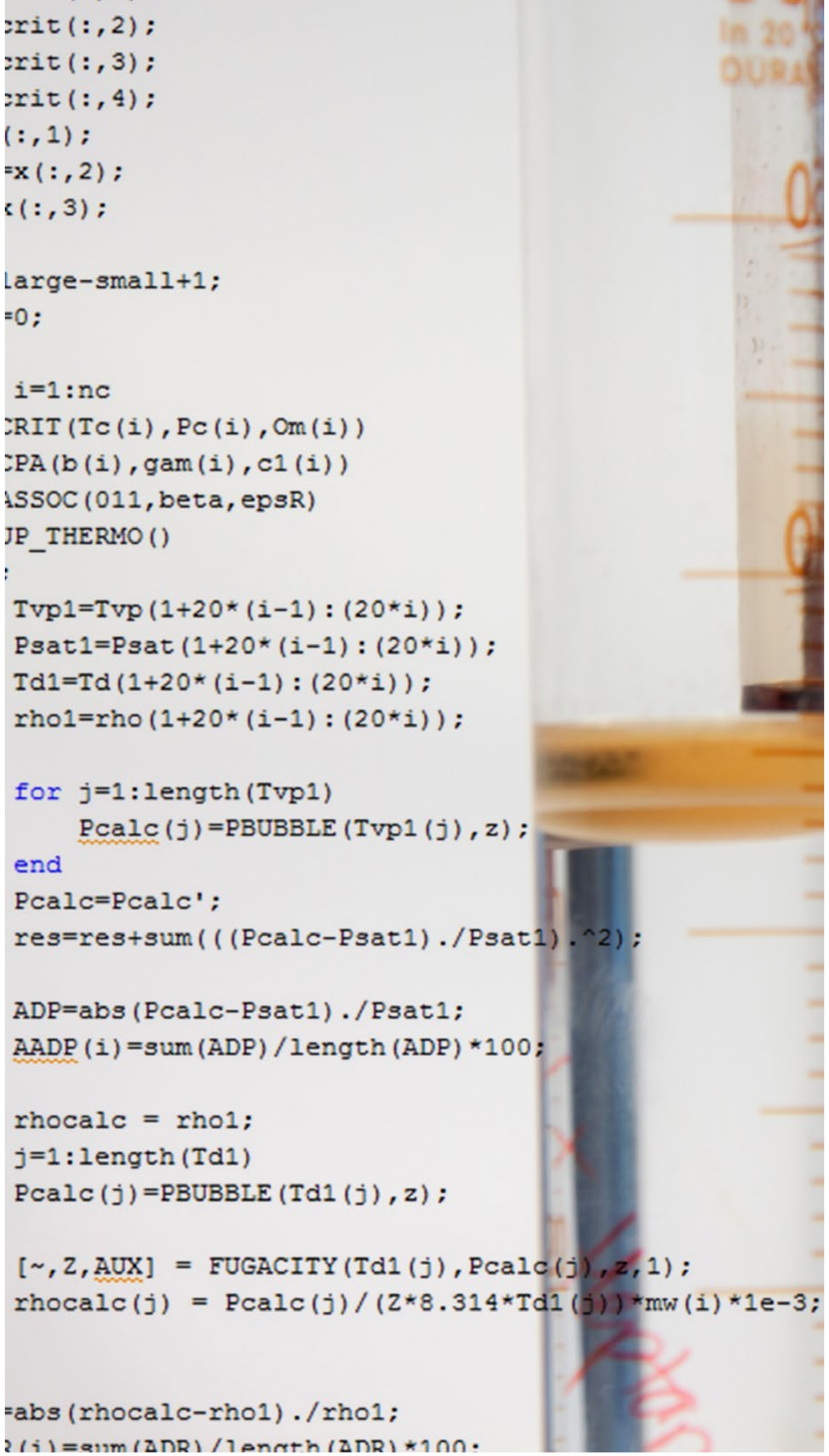


Feedback from Industry on CPA

Prompted by the 20 years anniversary of the model, CERE asked member companies in the Industry Consortium for their opinions on the CPA– and also for their expectations for the future development of this and other thermodynamic models. Below are the opinions of four representatives from CERE consortium member companies on the future needs for thermodynamic models and data.

"SAFT and CPA have been real breakthroughs in the modeling of thermodynamic behavior of fluid mixtures, and it is not surprising that a large majority of the thermodynamic community have turned to this new type of models. The main reason why I believe that we will have to continue working on these equations in the future is that they clearly show that it is possible to introduce molecular scale concepts in an industrial tool, thus making it possible to describe systems that contain a variety of complexities simultaneously (molecular asymmetry, electrolytes, high dilution, extreme conditions, derivative properties, …). As the fundamental framework of the equation is better than previous approaches, it becomes possible to extrapolate data (which remain crucially needed) with higher reliance, while in the past we were limited to correlating empirical parameters. Future developments have to strengthen the achievements by improving predictive parameterization concepts (i.e. group contributions) for complex systems that are often encountered in industry, specifically material from biological origin (multifunctional highly branched molecules dilutes in various solvents, including mixed solvent electrolytes). The effort from the academic community will consist in making sure that (1) the systems investigated correspond to industrial needs; (2) systematically compare the conventional models with the new approaches so as to point on the advantages; (3) whenever possible, make available tools that include equations + parameters for an easy accessibility of the results."

"Twenty years ago, the handling of aqueous components at high pressure was a challenge for the oil industry. CPA is a very valid contribution to solve that issue. For many years the industry has used cubic equations for gas and oil mixtures. A model that in the absence of aqueous components reduces to a cubic equation is highly appreciated. Looking forward models and algorithms are needed, which with a unique set of parameters can handle mixtures of gas, oil and aqueous components over wide ranges of pressure, beyond 2000 bar, and temperature, above 200°C. The mixtures might precipitate solid or solid-like phases as for example wax, salts and asphaltenes. Only few laboratories can measure complex non-standard fluid data at such high pressures and temperatures. That could be an area for CERE to prioritize. It would also be interesting to see CERE tackle fluid transport challenges like wax deposition in subsea pipelines and asphaltene deposition in oil wells."

"The problems we are dealing with are related to the phase equilibrium of both classical and more "modern" mixtures, which we see in our processes. The problem of efficient separations is always relevant, as well as the problem of consistent phase equilibrium and chemical equilibrium calculations. Modeling of systems with electrolytes and biomolecules can be also mentioned. In the latter case, methods for pure components' properties estimation are missing sometimes. Even if they are there, their reliability is sometimes unknown. Solubilities of gases also constitute a topic that comes now and then, as we can only rely on data and they are not always there."

"Just a few headwords on what I expect from the next 20 years of research at CERE: Development of more "ab initio" thermodynamic models, meaning model parameters derived from the well-known atomistic/microscopic nature of the molecules. Development of more comprehensive models, meaning a single model should be able to predict the whole bunch of thermodynamic properties. Development of models with a broader application range, meaning that models should be applicable from gases to non-aqueous electrolyte solutions in a broad range of temperatures, pressures and concentrations. Experiments to develop and prove the validity of the above models. Educating excellent students!"

Mauro Torli and Philip Fosbøl discussing process optimization possibilities.

A flexible Approach to Bio-energy

Coordinated by CERE, an international consortium will take energy production from biomass to the next level. The key idea is to combine thermochemical and biological processing of biomass in order to provide the optimal solution at any given time depending on market conditions.

Presently, bio-energy can be divided into either production of bio-fuels or production of heat and power. These sub-fields have separate technology, and separate stakeholders both on the academic and industrial side. However, the time has come to merge the two fields.

"Our idea is to create a technology platform able to produce a combination of biofuels and heat plus power. Depending on market conditions the balance between the two types of production can be shifted to always yield the optimal solution," says Associate Professor Philip L. Fosbøl, coordinator of one of the work packages in SYNFERON, an ambitious international consortium led by CERE.

Due to both climate protection and energy independency concerns, several governments have included bio-energy in their policies. This is very much true in Denmark, where biomass and wind power currently are the two main renewable energy focus areas.

Today, bio-energy roughly follows two different routes. In one of them, biomass is the starting point for catalytic production of "syngas", which is a mixture of H_2, CO_2, and CO. The syngas is used in combined heat and power production. In the second path, biomass is fermented to yield ethanol or similar substances which may be used as biofuels.

Fermentation of "syngas" increases flexibility

In the SYNFERON project (Optimized SYNgas FERmentatiON for biofuels production) syngas is to be fermented to liquid (alcohols) and gaseous (methane) biofuels by mixed microbial solutions.

"By merging the combined heat and power production with fermentation of the syngas, the processing of syngas can always follow the optimal path. That is, the final production will be easily diverted to combined heat and power or to biofuels satisfying thus the supply and demand of the biomass and energy markets. For example, when the heating demand is high, the syngas will mainly be exploited through combined heat and power production, but when the heating demand is low, the syngas will be fermented to storable liquid or gaseous biofuels."

SYNFERON brings together four research groups at DTU Chemical and Biochemical Engineering (CERE, CAPEC-PROCESS, PILOT Plant, BioEng), one technological consultancy and development company (Danish Gas Technology Centre), two companies in the separation process area (Aquaporin and Biosystemer), one gasification company (Agnion Energy, Germany), and one academic partner in biomass gasification and syngas fermentation (Bioeconomy Institute, Iowa State University, USA).

The role of process optimization

In order to achieve an efficient fermentation of syngas, a number of technological advances need to be made. These include novel bioreactors, pressure control, and use of suitable surfactants for increased gas/liquid mass transfer efficiency. Also, biomimetic membranes and diabatic distillation for gentle and cost-efficient purification of liquid biofuels are to be utilized.

These tasks will all be carried out by other consortium partners, while CERE will undertake overall coordination and process design optimization.

"As the partners produce scientific and developmental results, our role will be to gather all this new information and make sure that we have a common understanding within the consortium, ensuring that we all continue to move in the same direction," says Philip L. Fosbøl.

Overall SYNFERON coordinator is CERE Chairman Professor Georgios Kontogeorgis, while Philip L. Fosbøl coordinates the work package "Engineering analysis of the proposed platform".

"Process optimization will be very important. For instance, if you ferment syngas into ethanol you will normally achieve an ethanol content of 3-5 %, which is way too low for biofuel purposes. Achieving a higher concentration is easy enough, but you need to be very focused on your energy consumption in that process, as this will be absolutely crucial for the economic feasibility."

Conventional technology does not allow for production of pure ethanol.

"The thermodynamics of the process sets 96 % ethanol content as the natural ceiling. Routes around this problem have been found, but again one needs to be highly aware of costs. It will always be a balance between the ideal solution and economic feasibility."

A surge in bio-energy interest

Another task in the same work package will be comparison with other biofuel technology solutions.

"This is actually very important. During especially the last five years, we have seen a real surge in the interest in bio-energy. We need to be careful not to duplicate the works of others. We don't want to waste our time on something that others have already developed - and have maybe even patented already," Philip L. Fosbøl states.

Further, CERE is responsible for simulations.

"Initially we will use existing, commercial software. Later we may have to develop new software ourselves. For instance, this could be in the form of a new module for integration into Aspen Plus. This will all depend on how the project evolves. How well will existing software perform when applied to the new processes? And how do the consortium partners envision the direction of the project?"

The SYNFERON project is co-financed by Innovation Fund Denmark. The grant of 2.3 million EUR plus additional funding from the partners guarantees at least three more years of the consortium. This may sound like a rather long time frame, but considering the ambitions this is not the case, Philip L. Fosbøl underlines:

"When the grant expires we want to have a technological solution. We may not become ready for pilot scale implementation, as the challenges are complex, but we will make it to a demonstration state – meaning a process that would work in bench scale, not just in laboratory scale."

Forward this article

Georgios Kontogeorgis, Professor

Philip L. Fosbøl, Associate Professor

Mauro Torli, PhD student

Supplementing Existing Biogas Expansion

The ultimate objective of the SYNFERON project is the development of a gasification/biosynthetic technology platform. This will include both a novel reactor type, development of designated microbial mixtures for the purpose, and energetically favorable and thus cost-efficient downstream processing for liquid fuels by combining biomimetic membranes and diabatic distillation. The project complies with the Danish Energy Policy for further development and commercialization of Danish strengths within Bioenergy. The existing biogas industry in Denmark is expected to grow significantly. The SYNFERON technology platform will supplement the existing production of biogas, as this technology would enable the utilization of dry biomass, which is not suitable for conventional anaerobic digestion. This additional biomass resource would be enough to supply several hundred SYNFERON-type plants with a cumulative capacity of about 3-8 GW. This would cover a significant percentage of Danish energy demand while creating several thousand new jobs. Also, the implied increase in the use of residues – including sewage sludge and wastes – can provide an extra income to farmers and/or solve waste treatment problems.

The SYNFERON project

Partners in the SYNFERON project (Optimized SYNgas FERmentatiON for biofuels production) are: CERE, CAPEC-PROCESS, PILOT Plant, BioEng (all research centers at DTU Chemical and Biochemical Engineering), Danish Gas Technology Centre, Aquaporin, Biosystemer, Agnion Energy (Germany), Bioeconomy Institute at Iowa State University (USA). Of the initial total budget of 2.8 million EUR, 2.3 million EUR is financed by Innovation Fund Denmark, while the partners contribute with the remaining 0.5 million EUR. CERE Chairman, Professor Georgios Kontogeorgis coordinates SYNFERON. The project duration is four years, ending by early 2019.

New Project on Biogas Upgrading

Biogas is set to play a leading role in the energy systems of several countries including Denmark. Associate Professor Philip L. Fosbøl, CERE, has received a grant for a joint industry project aiming at upgrade of biogas. While natural gas is 100 % methane, biogas contains roughly 65 % methane and 35 % carbon dioxide. The aim of the new project entitled BIOCO2 is to develop and test a new efficient way of upgrading biogas for combined production of bio-methane and CO_2. Even though CO_2 is a highly problematic greenhouse gas, it is also an important commodity for a number of industries, e.g. the food and beverage industry, the pharmaceutical industry, and the welding and metal industry. Thus, there is potential for using the captured CO2 from biogas-upgrading as a replacement of manufactured CO_2 from fossil fuels. Besides contributing to sustainability, the technology may improve the economy for biogas producers, both by reducing energy consumption and by providing an additional source of income; namely high-quality CO_2. The BIOCO2 partners are CERE, Union Engineering, and Danish Gas Technology Centre. The project has a total budget of 1.9 million EUR. It is funded by the Danish Energy Agency's Energy Technology Development and Demonstration Program (EUDP) and is scheduled to run from 2016-2020.

Close CERE-DHRTC Collaboration

Inaugurated in 2015, the Danish Hydrocarbon Research and Technology Centre (DHRTC) is now well established at the DTU Campus in Lyngby. While DHRTC is a national center with ties to five academic institutions, CERE is a natural partner and currently engaged in a suite of joint projects.

"We have already carried out a series of mutual projects with relatively short duration. Additionally we have several ongoing such projects, and we hope to be able to announce the first major collaborative venture quite soon," says Associate Professor Nicolas von Solms, who is a member of the CERE faculty but has a special role in relation to the new center, which is dedicated to applied oil and gas research of relevance to the Danish North Sea.

"I would like to underline that my role as DTU Local Focal Point in relation to DHRTC is not just to represent CERE. I think of myself as an active matchmaker for new collaborations across the entire DTU. Any center or department at DTU will be able to suggest projects with possible DHRTC collaboration, just as I am actively trying to find relevant partners across DTU when a call for partners is about to come up," Nicolas von Solms stresses. "I maintain a list of relevant competencies across DTU, and it is not just kept in my drawer but presented to DHRTC frequently on relevant occasions."

The five academic partners of DHRTC are 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.

"We meet with DHRTC once every fortnight, and the meetings are not always in Lyngby, but can also be at the other institutions," Nicolas von Solms explains.

In 2016, CERE took part in six collaborative projects with DHRTC of shorter duration, typically of about three months each. Subjects were: analysis of formation damage by contaminated injected water (Associate Professor Alexander Shapiro); thermodynamic analysis of oilfield scale and corrosion (Associate Professor Kaj Thomsen); effect of particle size on emulsion formation in smart water enhanced oil recovery (Associate Professor Kaj Thomsen); under deposit corrosion (UDC) mechanisms (Associate Professor Philip L. Fosbøl); solubility measurements of corrosion products (Associate Professor Philip L. Fosbøl); evaluation of the impact of compositional characterization of reservoir fluids on modelling (Senior Researcher Wei Yan).

Furthermore Associate Professor Kaj Thomsen will advise a two-year postdoc position in collaboration with DHRTC on a project titled "Thermodynamic modelling of Smart Water".

Also, two shorter postdoc projects looking at thermodynamic measurements and modeling in systems relevant to DME (dimethylether) flooding will commence shortly. The new postdocs will work with Senior Researcher Wei Yan, Associate Professor Nicolas von Solms, and Professor Georgios Kontogeorgis.

"Finally, CERE is happy to supply DHRTC with support from our skilled technical personnel upon request. Currently, DHRTC draws on technical services equaling approximately one full-time technician over the year, and compensates us accordingly. Overall, it is fair to say that DHRTC contributes significantly to the activities of CERE," ends Nicolas von Solms.

Forward this article

Software for Electrolytes, Asphaltenes, CO_2

CERE is happy to provide industry consortium members and other partners with software for thermodynamic modelling. The products are gradually improved both in functionality and user-friendliness. Moreover, several new tools were added to the suite in 2016.

PhD student Anders Schlaikjer demonstrating his eCPA to his colleagues Xiaodong Liang and Alay Arya.

Chemical engineers in both academia and industry are able to enjoy a suite of software products developed and maintained by CERE. The researchers at CERE use various home-brewed types of software especially within thermodynamic modelling. Some years ago, CERE decided to turn these in-house tools into products with broader application by investing the necessary resources in user-friendliness and verifications. In 2016, several new tools were added to the suite.

The "CERE ExpertThermo" enables the presentation of results from phase-equilibrium calculations as tabular formats and graphical plots, which can be obtained and understood without the need of programming skills.

"The new software integrates several tools developed over a large span of years by Michael Michelsen (former Professor at CERE, who retired in 2015, editors' remark), and also by other staff at CERE. This is an effort we have undertaken over some years. Now we are ready to pass it on to the CERE Consortium members and others in the chemical engineering society," says Associate Professor Philip L. Fosbøl, lead developer for CERE ExpertThermo.

CERE ExpertThermo combines a multi-component database with a set of chemical properties. Also, it integrates several thermodynamic models and algorithms which allow for P-xy, T-xy, ternary, phase-envelope diagrams and flash calculations plus many other types of basic analysis. CERE ExpertThermo is built on a set of compiled Fortran dynamic link libraries for use in Matlab. The software can also be seen as a DLL outside Matlab. Matlab is a widely used engineering and programming language for numerical computation and visualization.

"Matlab makes problem solving and programming relatively easy for a chemical engineer without involving high programming skills. By integrating CERE ExpertThermo into Matlab, the results can be further processed and shown in depth using other mathematical and plotting tools offered by that platform," says Philip L. Fosbøl. "Consequently, the new product provides an advanced approach to thermodynamic modelling as it is the chemical engineer who decides what functionalities his script will implement. In other words it opens the door to a wide range of new functionalities."

Prediction of asphaltene precipitation

Another addition to the suite of CERE software products is a new tool for calculating asphaltene precipitation.

"Asphaltene precipitation has been a flow assurance problem in the oil industry for several years. There are a few commercial software products available, but their reliability is not established. Therefore we, at CERE, have created the Asphaltene Matlab tool," says Alay Arya, who is a PhD student at CERE. The new software is based on his PhD project.

"The Matlab environment is user friendly both in terms of input and in terms of results in either tabular form or as plots. It also gives the user the flexibility to study the results by modifying different model parameters," Alay Arya continues.

The basic thermodynamic models – Cubic Plus Association (CPA) and Pertubed Chain Statistical Associated Fluid Theory (PC-SAFT) were prepared by CERE in Fortran code years ago. The Asphaltene Matlab tool accesses these basic models through Matlab executable files, also known as MEX files.

"The tool has been validated with respect to several case studies available in the literature. It has been disseminated to the Consortium member companies which participate in the CHIGP joint industry project and is being used. We, at CERE, believe that the tool is very useful for the oil industry especially in relation to enhanced oil recovery by gas injections where the effect in relation to asphaltene precipitation can be simulated before implementation in the field," ends Alay Arya.

The CPA model extended to electrolytes

A further development is software for the modeling of mixtures containing electrolytes. Electrolytes are characterized by the presence of ions either in solution or in salts, and simulation of systems containing electrolytes is relevant to a wide range of industrial applications.

"It is impossible to model the behavior of electrolyte systems by the use of traditional equation of state based models. Besides the standard interactions between molecules, the presence of ions means that also electrostatic forces will be at play. These forces have effect over longer distances than the "classic" molecular forces," explains PhD student Anders Schlaikjer.

The new software is based on a new model, the eCPA, which is an extended version of the Cubic Plus Association (CPA) model.

"The model reduces to its original form, the CPA, when no electrolytes are present, while the new functionalities come in at the presence of electrolytes," Anders Schlaikjer explains. "This is a considerable advantage, as one can use already existing CPA parameters for all other substances than the electrolytes."

The eCPA has been successfully tested for a range of systems.

Better simulation of CO_2 capture

Besides the introduction of new tools, other CERE software products are steadily being improved. For instance, the "CAPCO2" programme for carbon capture calculations has been significantly extended during 2016.

"The programme is able to handle a larger range of carbon capture solvents, and also promoted technologies," explains Philip L. Fosbøl, lead developer for CAPCO2.

Traditionally, amine based solvents have been preferred in practical carbon capture, but recent years have seen interest in many different types of alternative solvents.

Carbon capture involves a basic dilemma. For the actual capture one would like to have a solvent which binds strongly to the carbon, as this would enable a fast process running with a small amount of solvent at a limited size plant. However, the drawback soon becomes evident, as the bonding needs to be broken in order to obtain pure CO_2 and also regenerate the solvent. If the bonding is strong, it will take a large amount of energy to break it, which will be costly and the process becomes non-feasible and unsustainable.

"A way to overcome this dilemma could be to take a "slow" solvent, involving low energy consumption, and speed it up by adding promoters to the process. This is a promising approach, but it is also demanding in terms of calculation, as complexity is increased," Philip L. Fosbøl notes. "We have extended CAPCO2 to keep up with these developments."

CAPCO2 is easy to use as it is Aspen Plus process simulation compatible. The programme builds on the Extended UNIQUAC model. Benchmarking in European projects has shown CAPCO$_2$ to be at least as accurate as the best programmes available from other research groups. For instance, the software can be used for calculating the cost per volume of CO_2 captured. Further, one can see how large the unit will need to be in order to capture the desired amount of CO_2. Also, CAPCO$_2$ can calculate the energy consumption for a suggested new facility.

Forward this article

Anders Schlaikjer, PhD student

Alay Arya, PhD student

Georgios Kontogeorgis, Professor

Xiaodong Liang, Assistant Professor

Philip L. Fosbøl, Associate Professor

NEWS
from CERE

Prize for Enzyme Carbon Capture

CERE PhD student Arne Gladis received first prize in an innovation contest during the annual Research Day of the Department of Chemical and Biochemical Engineering at DTU. 30 PhD students took part in the competition, which was held on May 27.

Arne Gladis' winning entry was a poster entitled "Can enzymes save the world's climate?" Supervised by Associate Professor Nicolas von Solms and Professor John Woodley, Arne Gladis works on enzyme enhanced CO_2 absorption rate-based modeling and pilot plant validation. The aim is to improve CO_2 absorption in solvents that can be regenerated with low energy by means of enzymes.

Also in 2016, Arne Gladis took part in the 13th International Conference on Greenhouse Gas Control Technologies held in Lausanne, Switzerland, 14-18 November, joining two other CERE researchers, Associate Professor Philip L. Fosbøl, and recently graduated PhD Jozsef Gaspar.

CERE Chairman visits China and Mexico

Future collaborations were the prime topic during a visit 1-7 May by CERE Chairman Georgios Kontogeorgis to Xi'an Jiaotong University, Xianyang, China.

Professor Kontogeorgis gave a short course on advanced thermodynamic models and visited the facilities of the thermodynamics groups. He was also appointed Adjunct Professor to Xi'an Jiaotong University. Host of the visit was Associate Professor Xiaopo Wang, and the stay was sponsored by the National Natural Science Foundation of China.

On November 8-13, Professor Kontogeorgis visited the Technical University of Mexico (Instituto Polytecnico National, IPN), Mexico City. He gave a plenary lecture on applications of thermodynamics for sustainable chemical engineering with emphasis on energy. Further, he discussed collaborations between IPN and DTU.

High Priority for Product and Process Design

No less than five representatives from CERE attended the 14th International Conference on Properties and Phase Equalibria for Product and Process Design (PPEPPD). Held in Porto, Portugal, on 22-26 May the conference attracted a total of 311 participants from 36 countries.

CERE was represented by Chairman Georgios Kontogeorgis and PhD-students Alay Arya, Christos Tsanas, Anders Schlaikjer, and Andre Vinhal.

The conference featured presentations on topics like quantum mechanics, molecular dynamics and phase equilibria with applications in a range of fields including oil, biomass, polymers, and pharmaceutical development.

"The broad range of topics allowed constructive discussions between people of different areas of thermodynamics. Also noteworthy was the good balance between academia and industry," says Andre Vinhal, who was a debutant at the conference. "The participation has already affected my work, as many of the ideas and suggestions from colleagues will be implemented in my research."

The PPEPPD is organized every 3 years, with the next event to take place in Vancouver, Canada, in 2019.

PetroPhase with a Touch of Shakespeare

CERE co-organized the 17th International Conference on Petroleum Phase Behavior and Fouling – or PetroPhase.

The annual event is where industry and academia dedicated to the study of properties and chemistry of petroleum fluids and their effect on producing, processing, and refining in the upstream, midstream, and downstream industries meet. The 2016 version was chaired by Associate Professor Nicolas von Solms, Senior Scientist Wei Yan, both CERE faculty members, and Dr. Simon Andersen of Schlumberger.

180 people attended and more than 150 technical presentations were given. The conference was held on 19-23 June in Helsingør. The participants were able to enjoy a gala dinner held in Kronborg Castle, which is also the prime venue for William Shakespeare's famous play "Hamlet". In fact, the (late) Danish prince Hamlet even made an appearance during the dinner!

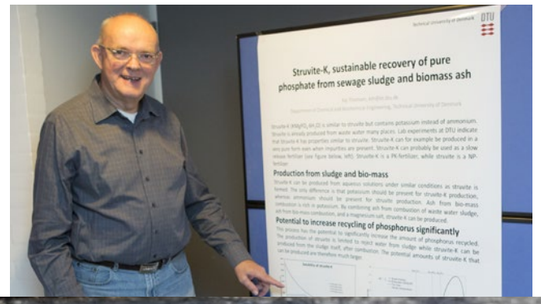
Phosphorus in the Circular Economy

Associate Professor Kaj Thomsen and Center Coordinator Hanne Pernille Andersen represented CERE when the first Nordic phosphorus conference was held in Hyllie, Sweden, on 27-28 October.

Participants included academia, the Nordic countries' water and waste water treatment organizations, industry, and environmental authorities.

The idea behind the conference was to create a meeting place for exchange of knowledge on better utilization of phosphorus in a "Circular Economy" where waste is turned into raw materials.

Highly relevant to the scope of the conference, Kaj Thomsen presented his poster "Struvite-K, sustainable recovery of pure phosphate from sewage sludge and biomass ash". The poster describes a new method for the recovery of phosphorous from sewage sludge and fly ash. Hopefully, the method will be developed on a larger scale in the future.



Evaluation of Master Program in Petroleum Engineering

In 2016, the Master program in petroleum engineering at DTU successfully passed an extensive evaluation. The process started at the end of 2015 and ended in November 2016. All educational programs at DTU undergo these evaluations every few years. The multistage procedure involves a report prepared by the head of studies followed by evaluation from an external committee consisting of the leading authorities in the field; comparative mutual evaluation of two other Master programs passing the evaluation process simultaneously; and the production of a paper on visions for future developments which is then discussed with the leadership of DTU.

While the Master program started as a marginal activity with just a few students, it has evolved into a large educational program provided by DTU with around 45 students joining each semester. Several CERE faculties teach.

The program received a highly positive evaluation, especially noting the rapid development, the high international level, and the popularity among the students. Head of studies for the program is Associate Professor Alexander Shapiro.

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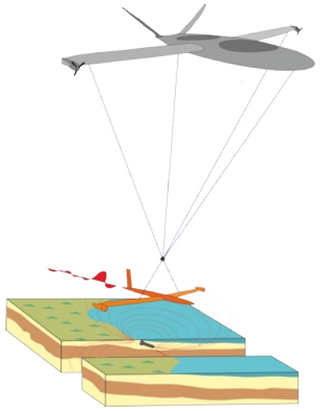
NEWS from CERE



Drones carry out Magnetic Surveys

Unmanned Aerial Vehicles (UAV's), also known as drones, may find a future in magnetic surveys relevant to the discovery of new energy resources. Geophysicist Arne Døssing, Senior Researcher at DTU Space and member of the CERE faculty has received funding for a new project on UAV's for high-quality magnetic surveying. Magnetic surveying from UAV's may be relevant to a range of applications such as finding unexploded mines at land or sea, necessary before cables for new offshore windfarms can be laid, for instance, and in the discovery and exploration of mineral or energy resources such as oil and gas, as well as geothermal reservoirs. External project partners are Sky-Watch, Geo, DONG Energy, and Royal Danish Navy EOD Service. Funding is provided mainly by Innovation Fund Denmark. The UAV-QMS project is due to commence in the spring of 2017 and has a total budget of 16 million DKK.

An Evening of Petroleum Engineering

On 23 November, DTU hosted the meeting of the Copenhagen section of the Society of Petroleum Engineers (SPE), organized by CERE. The SPE Copenhagen section, among other activities, organizes monthly SPE meetings. These meetings are being organized by the different petroleum companies operating in Denmark and occur at different places around Copenhagen. Once a year, such a meeting is traditionally hosted by DTU. Around 90 participants were registered for this year's meeting.

Several CERE faculty members presented the status on their respective fields.

Associate Professor Alexander Shapiro presented new knowledge on particles in pores. Fine particles appear naturally in petroleum reservoirs, and may be released by injection of brine with modified salinity – also known as smart water flooding. Alexander Shapiro and his group study the behavior of these particles, which – depending on circumstances – can be either beneficial or harmful in relation to petroleum engineering.

On a related subject, Associate Professor Kaj Thomsen showed how changes in pressure or temperature, and mixing of incompatible brines can cause mineral precipitation in oil fields and production equipment. His message was that mineral precipitation should not always be considered a problem, but may sometimes contribute to increasing the oil recovery factor.

Further, Professor Ida L. Fabricius discussed how pore-fluids influence the stiffness and strength of chalk, which is the major sedimentary rock type in the oil and gas reservoirs in the Danish North Sea. Ida L. Fabricius coordinates the Geophysics Research Group at DTU Civil Engineering.

Finally, Professor Erling H. Stenby, Scientific Director at the Center for Oil and Gas (DHRTC), presented the activities at DTU on Enhanced Oil Recovery (EOR). Erling H. Stenby, who previously was head of CERE for 20 years from 1994, guided his audience through the development of oil and gas research at DTU during decades of changes in political agendas, strong fluctuations in the price of oil, etc. The evening also included a dinner and a student poster session.

Fluid Theories in Process and Solvent Design

Predictive thermodynamic models allow new concepts in simultaneous product and process design. At a seminar on April 14, Joachim Gross, University of Stuttgart, Germany, showed applications of simultaneous solvent and process design for a high-pressure CO_2-absorption process. The simulations were based both on the PC-SAFT thermodynamic model and on classic density functional theory (DFT). Results were presented for vapor-liquid and liquid-liquid interfacial properties, as well as for fluids in confined space (porous materials). Joachim Gross is Professor, Dr.-Ing. at the Institute of Thermodynamics and Thermal Process Engineering, University of Stuttgart.

CERE Seminars by Distinguished International Speakers

How Water Flooding may Weaken Chalk

Sinking platforms are the ultimate consequence of the serious seabed subsidence which may be caused by the so called water weakening effect. The effect, which can be seen when oil reservoirs are flooded with seawater to drive out more oil, was the topic of a seminar given by Aksel Hiorth, University of Stavanger, Norway, on February 25. Professor Hiorth was able to present new insight gained from both lab experiments and numerical modelling. One of the main conclusions was that the effect is most likely related to chemical interactions between the rock and injected water. Aksel Hiorth is Professor within reservoir technology at the University of Stavanger, and also Research Director at the National IOR Centre of Norway.

Management of Scales in Oil Reservoirs

While scaling is a well-known challenge in oil production, it is a relatively new approach to simulate the underlying reservoir processes. At a seminar held March 11, Eric Mackay of Heriot-Watt University, Scotland, presented reservoir simulation and reactive transport models which can be used to better understand the impact of reservoir processes on oilfield scaling. His key message was that such calculations allow identification of the severity of the potential scaling regime, and to quantify the impact of the scaling problem. Eric Mackay holds the Foundation CMG Chair in Reactive Flow Simulation in the Institute of Petroleum Engineering at Heriot-Watt University. Further, he is a Principal Investigator for the Flow Assurance and Scale Team Joint Industry Project.

Courses at PhD Level

CERE has a history of hosting advanced courses on thermodynamic models for its own PhDs and industry. 2016 was no exception with the "Advanced Course on Thermodynamic Models: Fundamentals & Computational Aspects". Companies and academic institutions from 8 countries were represented among the 25 participants. Main lecturer was Senior Researcher Wei Yan, DTU Chemistry.

Also held was a PhD level course on "Electrolyte Solution Thermodynamics" with Associate Professor Kaj Thomsen, DTU Chemical and Biochemical Engineering, as main lecturer. Four PhD students attended the course, which focused on experimental methods for measuring properties of salt solutions, molecular interactions in electrolyte solutions, di-electric properties of solvents and their effect on salt solubility, and a number of other properties for electrolytes including equations of state and volumetric properties.

Read more on our website

NEWS
from CERE

To Err is Human, but potentially Costly

Formerly with Royal Dutch Shell, Ronald McLeod has more than 30 years of industry experience. Based on his book "Designing for Human Reliability: Human Factors Engineering for the Oil, Gas and Process Industries" he gave a seminar at CERE on October 27. At Shell, Ronald McLeod was Global Discipline Lead for Human Factors Engineering. He has a background in psychology. During his presentation at DTU he tried to explain what may have occurred in the minds of operators involved in major incidents. Further, he showed how certain psychological processes can lead people to make decisions and to take actions that otherwise seem impossible to understand. Not surprisingly McLeod's provocative headline for the event "The Problem with People: Why do we make perverse decisions?" attracted quite a crowd and led to a lively debate.

Oil adheres to porous surface | Introduction of GreenZyme | Surface wetted and oil released

Smart Enzymes for Oil Recovery

A new commercial enzyme product is able to increase the recovery rate in oil and gas production. This is according to Lucas Evangelista of Biotech Processing Supply, Argentina, who presented his company's product GreenZyme during a CERE seminar on November 18. The product is based on a water soluble liquid enzyme designed to interact catalytically with hydrocarbons. GreenZyme is made with DNA of oil loving microbes where the oil digesting property is neutralized, but where the ability to attach to and release hydrocarbons is kept. After the release of hydrocarbons from pore walls in the reservoir, the enzymes will be attached to the solid surfaces and dissolved in the water phase in the reservoir. Here, the enzymes are available to interact with new hydrocarbons and continue to cause release of oil.

Molecules Functionalized for Oil Recovery

Addition of small amounts of functionalized molecules may increase efficiency in oil and gas recovery drastically. This was the key message as Professor Abbas Firoozabadi of Yale University, USA, inspired CERE staff and students in a seminar on November 9. His title was "Molecular structure in petroleum fluids and petroleum-interfaces in relation to flow assurance and improved oil recovery". Professor Firoozabadi showed how the inhomogeneity and structures of different molecules found in both petroleum fluid-aqueous phase and petroleum fluid-rock systems may have profound effect on hydrocarbon energy production. The presentation covered both experiments and molecular modeling, and led to the conclusion that improved oil and gas recovery can be achieved by changes in fluid structure and rock surfaces using small amounts of surfactants.

Highlighted Publications

The academic results from CERE are published in numerous scientific papers. It is not possible to mention all here (the full list is found in the electronic version of this report at CERE's website), but still, a few highlighted publications:

Screening of Ionic Liquids for dissolving Cellulose
The purpose of dissolving cellulose is to create new materials such as conductive fibers that can replace metal wires for conducting electricity. In her research project at DTU Chemical and Biochemical Engineering PhD student Yanrong Liu measured the solubility of cellulose in seven different ionic liquids. She also used the COSMO-RS model for predicting the solubility of cellulose in 357 different ionic liquids. The work was published as a cover paper entitled "Predictive Screening of Ionic Liquids for dissolving Cellulose and Experimental Verification" in Green Chemistry, volume 18, number 23, pages 6147-6398, 2016.

Applied Colloid and Surface Chemistry
Lotions and many similar personal care products are complex emulsions. This is just one of many examples of colloid and surface chemistry from everyday life. This type of chemistry also has implications in a wide range of industrial sectors, ranging from coatings and materials to medicine and biotechnology. In their book "Introduction to Applied Colloid and Surface Chemistry", Professor Georgios Kontogeorgis and Associate Professor Søren Kiil, both DTU Chemical and Biochemical Engineering, explain the topic to professional readers such as chemists, chemical engineers, biologists, material and food scientists, etc.

New PhD Projects

"Rock Mechanics and Fluid Saturation Study"
PhD student: Leonardo Teixera Pinto Meireles. Supervisors: Ida L. Fabricius, Michael Welch. Funded by DHRTC.

"Thermodynamics of Petroleum Fluids relevant to Subsea Processing".
PhD student: François Krüger. Supervisors: Nicolas von Solms, Georgios Kontogeorgis. Funded by Statoil and DTU Chemical and Biochemical Engineering.

"Thermodynamics, Design, Simulation and Benchmarking of Biofuel Processes"
PhD student: Mauro Torli. Supervisors: Philip L. Fosbøl, Georgios Kontogeorgis. Funded by Innovation Fund Denmark and DTU Chemical and Biochemical Engineering.

"Thermodynamics Modeling of CO_2 Gas Hydrate Formation Systems"
PhD student: Sun Li. Supervisors: Georgios Kontogeorgis, Xiaodong Liang. Funded by the Chinese Scholarship Council and DTU Chemical and Biochemical Engineering.

"Phase Behavior of Inhomogeneous Fluids"
PhD student: Edgar Luis Camacho Vergara. Supervisors: Georgios Kontogeorgis, Xiaodong Liang. Funded by DTU Chemical and Biochemical Engineering.

Read more on our website

PhD Defenses

Petrophysical Aspects of Smart Water Flooding

Konstantina Katika, PhD.
Currently with Labster.com

Full title:
"Rock Physics of Reservoir Rocks with Varying Pore Water Saturation and Pore Water Salinity"

Supervisor:
Ida L. Fabricius

The project was funded by DTU, Maersk Oil, DONG Energy, and the Danish Energy Agency as a part of the Smart Water project.

Direct link to this PhD thesis

Water flooding is widely used to increase production during oil recovery. In "smart water flooding" water with selected ions is injected to enhance production further. Various mechanisms have been suggested in attempts to understand why, smart water flooding works. It is obvious, that an accurate understanding of the mechanism(s) behind the effect would enable optimization and thus increase chances of success. The project investigates several possible mechanisms, while also introducing new methodology for such studies. Especially the value of low field NMR (Nuclear Magnetic Resonance) spectroscopy is shown.

The focus of the project is reservoirs in the Danish part of the North Sea, with chalk or greensand lithology.

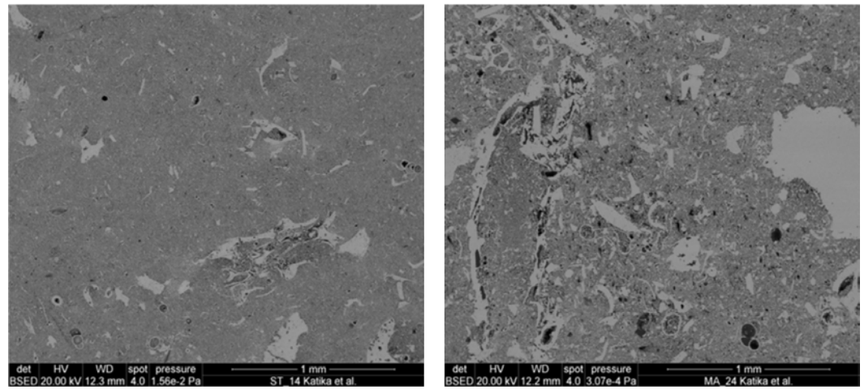
During core flooding experiments in the project, the rock was subjected to high temperature and external stress. Further, the fluid distribution within the pore spaces changes during the flow-through experiments and pore compressibility may change and solids precipitate in the pore space which may both reflect the situation during full-scale smart water flooding.

In order to investigate the interaction of pore water with selective ions on the solid/fluid interface, low field NMR spectroscopy, ultrasonic velocities, electrical resistivity, and mineralogical characterization were performed on reservoir cores.

Low field NMR spectroscopy was successfully used to identify changes in the surface-to-volume ration of chalk after the saturation with brines containing divalent ions. The technique was used successfully to detect the precipitation reactions that occurred among the magnesium, calcium and sulfate ions and carbonates, and thus formation of fines.

From rock mechanical testing, it was observed that divalent ions in high concentration affect the elasticity of the chalk. High salinity and especially potential determining ions (Mg^{2+}, Ca^{2+}, and SO_4^{2-}) soften the rock and promote pore collapse at lower stresses.

Development of novel methodology was an important objective of the project. Most notably, a low field NMR spectroscopy technique to determine small amounts of fluids, as they are produced during core flooding experiments was successfully developed. This technique was shown to be highly accurate for quantification of the oil fractions. Also, the technique provided accurate determination of the water fraction. Importantly, the water and oil face do not need to be separated.



Backscatter electron micrographs of chalk sample with mudstone texture (left), and chalk sample with wackestone texture (right) (Katika et al., I)

Towards Online Reservoir Management

Max la Cour Christensen, PhD.
Currently Postdoc at DHRTC

Full title:
"Multilevel Techniques for Reservoir Simulation"

Supervisor:
Allan P. Engsig-Karup

The project was financed through the Industrial PhD program at Innovation Fund Denmark with Lloyd's Register Consulting as primary sponsor.

Direct link to this PhD thesis

The combination of fast, powerful computers and recent advances in well control technology promises a bright future for optimization of oil and gas production. Ideally, feedback data during production will be processed in real-time to enable online corrections. However, this scenario depends on accurate predictions of porous media flow in a timely manner. The project addresses the challenge of improving speed and accuracy of simulation tools using multilevel algorithms and techniques for the purpose.

Simulation of the flow of oil, gas and water in the subsurface remains a challenging task with many uncertainties, which may affect the reliability of the resulting production forecasts. This may be caused by inaccurate numerical techniques, poor description of the physical processes, etc. Failure in predicting oil and gas production accurately may result in non-optimal decisions with a risk of very significant financial losses.

In many scenarios it can be beneficial to base important decisions on a sound statistical basis rather than a single deterministic calculation. A well-known method for providing such a basis is Monte Carlo simulations. However, as in a reservoir context one faces a 3D discretization of time-dependent nonlinear systems of partial differential equations, it quickly becomes impossible to carry out the required number of calculations with conventional approaches. One way to improve the efficiency of calculations where uncertainty is accounted for is by using coarse representations of the underlying model in a smart way. This is the underlying idea of Multilevel Monte Carlo (MLMC) simulations.

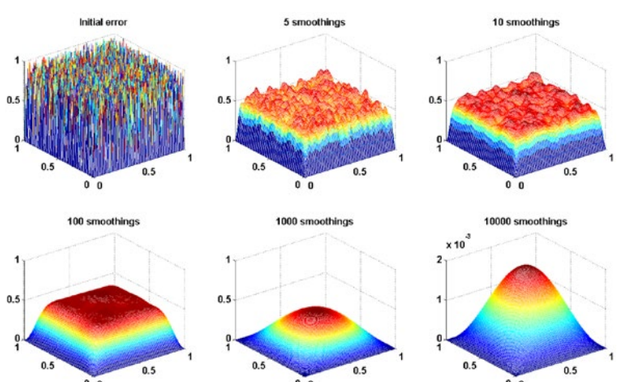
For example, using 60 processors as a cluster, MLMC was compared to standard Monte Carlo simulations. Here, MLMC converged in 8.5 hours, whereas standard Monte Carlo simulations needed 28.6 hours with the same level of accuracy.

The project presents a further improvement. Instead of up-scaling the coefficients of the partial differential equations, the very system of equations is up-scaled. This is achieved through application of a class of numerical up-scaling techniques. The method – referred to as the Full Approximation Scheme (FAS) - was shown to improve time-to-solution by having a larger basin of attraction, faster initial convergence, data locality and a lower memory footprint.

Even though the numerically up-scaled models were accurate, some diffusivity should be expected. Typically, the very coarse up-scaled models would underestimate the exact time, when water breakthrough occurs. Further, the choice of agglomeration had a large impact on the quality of the up-scaled models. It is important to leave the elements containing wells and their immediate neighbors un-agglomerated to capture the near-well flow accurately.

The proposed technique holds great potential in the acceleration of optimization techniques, where many realizations of the model are needed. For instance, it can be used to accelerate the optimization of well placements, water and gas sweeping patterns, etc. Furthermore, as wells become more advanced and allow more control of inflow/outflow in individual segments of the wells, an increased interest in real-time production optimization is seen. To accommodate this will require very fast simulation techniques.

Besides accelerated simulations, the project also looked at other fundamental approaches which are hidden for the end-user but nevertheless key to improve leverage of existing tools. These included possible optimization of linear solvers/preconditioners and non-linear solvers, alternative formulation and discretization methods, and finally, methods suitable for large-scale parallelization on large modern many-core clusters.



Gauss-Seidel smoothing on a Poisson problem with an initial guess containing random noise.

Smart Water Flooding in Carbonate Reservoirs

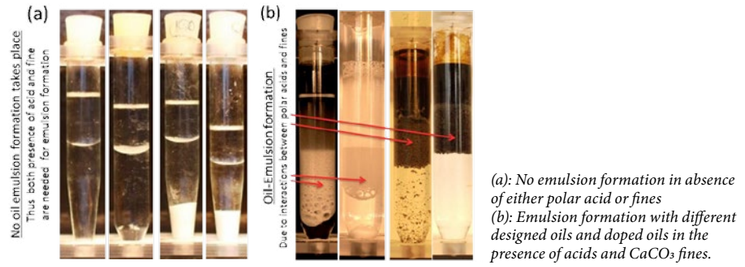
Krishna Hara Chakravarty, PhD.

Full title:
"Modeling of Salt Solubilities for Smart Water Flooding in Carbonate Reservoirs using Extended UNIQUAC Model"

Supervisors:
Kaj Thomsen, Philip L. Fosbøl

The project was funded by the Danish Energy Agency, Maersk Oil, and DONG Energy as a part of the Smart Water program.

Direct link to this PhD thesis



(a): No emulsion formation in absence of either polar acid or fines
(b): Emulsion formation with different designed oils and doped oils in the presence of acids and $CaCO_3$ fines.

Advanced water flooding – or "smart" water flooding – aims at increasing oil recovery by altering the composition of the injected brine. Specifically, the concentration of selected ions in the brine is changed. This is a low-cost, not-toxic enhanced oil recovery (EOR) method which has been shown to work in Middle East sandstone reservoirs. The project investigates the relevance of smart water flooding to carbonate reservoirs in the Danish part of the North Sea.

In the study, geochemical modeling of salt solubility at reservoir conditions was performed to explore correlations between different brine properties and corresponding increases in oil recovery.

Simulations based on density functional theory (DFT) show that ion substitutions on mineral surfaces can take place. The ion substitution causes an increase in Ca^{2+} concentration in the pore space. Thus, additional Ca^{2+} can change brine speciation and cause insoluble salt precipitation.

It is observed that crude oil interacts with insoluble salt to form water soluble emulsions. The composition of these emulsions was studied by gas chromatographic analysis. The availability of different soluble salts was shown to influence the level of emulsification. Ca^{2+}, Mg^{2+}, SO_4^{2-}, and PO_4^{3-} ions were observed to enhance oil emulsion formation considerably. Formation takes place only when insoluble fines and polar fraction are present in water and oil respectively. This emulsification therefore indicates an increased adhesion at the oil-water interface with release of residue oil from the mineral surface.

Speciation calculations using the Extended UNIQUAC model showed that the amount of fines formation was consistently correlated to the reported oil recovery for more than 128 core plugs. The correlation was consistent over variations in temperature, pressure, acid number, acid type, base number, aging temperature, aging time, formation water, composition, and core-plug wettability.

Further calculations showed that most brines are supersaturated at reservoir conditions when produced. The amount of insoluble salt existing (mobile fines) shows a one-to-one correlation to the reported EOR.

From extended UNIQUAC calculations it was observed that precipitation on injection takes place for most of the recommended brines. Injection brines which have been shown significant increase in oil recovery were also found to be supersaturated at reservoir/experimental conditions. Contrary to a proposed wettability alteration mechanism (suggested in the literature), speciation calculation at reservoir conditions showed no inverse correlation between the amount of precipitation and oil recovery. And for highly precipitating brines, also the amount of fines formation taking place (after ion substitution) showed good correlation to the observed increase in oil recovery. This shows a clear distinction between injected brine at room temperature and actually injected brine at reservoir conditions.

Experiments on reservoir core plugs from the Danish North Sea showed that pauses in water flooding can cause additional ion substitution and release of calcite fines from the mineral surface. The amount of released Ca^{2+} and CO_3^{2-}/SO_4^{2-} was beyond the solubility limit, indicating that insoluble $CaCO_3$ was produced due to attrition on the mineral surface. This attrition based fines production showed consistent correlation to the observed increase in oil recovery.

Based on this correlation, possible strategies have been developed for smart water flooding in different sections of the most oil producing fields in the Danish North Sea including the Dan field and the Halfdan field.

Advances in Post-combustion Carbon Capture

József Gáspár, PhD.
Currently Postdoc at DTU Compute

Full title:
"CO_2 Capture Dynamic and Steady-state Model Development, Benchmarking, Optimization, and Control: Applied to Piperazine and Enzyme Promoted MEA/MDEA"

Supervisors:
Philip L. Fosbøl, John Bagterp Jørgensen, Kaj Thomsen, Nicolas von Solms

The project was funded by DTU Chemical Engineering and the European Union's FP7 program as part of the OCTAVIUS project.

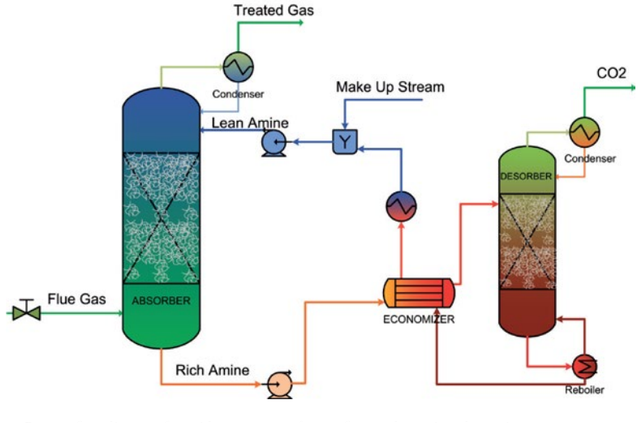
Direct link to this PhD thesis

Fossil fuels meet more than 80 % of the world's primary energy demand, and cause over 90 % of energy-related CO_2 emissions. Despite renewable energy investments in many countries, coal is projected to remain the largest source of power generation through 2040, and subsequently the largest source of CO_2 emissions. Carbon capture and storage (CCS) can potentially reduce these emissions. All necessary components of CCS technology exist, but reductions in operational costs are necessary for widespread implementation. The project investigates possible advances in post-combustion capture using alkanol-amine solvents, which is the most mature capture technology.

Amine based CO_2 post-combustion capture is a reactive absorption process involving a complex mechanism of simultaneously occurring reaction and mass transport phenomena. In the project a simplified mass transfer model was developed and applied to single and parallel reactions systems, i.e. MEA (monoethanolamine), PZ (piperazine), and MDEA (methyl diethanolamine). The model describes the acceleration of the mass transfer rate due to the reaction between CO_2 and amines. Afterwards, this sub-model together with the extended UNIQUAC thermodynamic model and correlations for physical properties was incorporated in a rate-based model for CO_2 absorption and desorption. The model results were benchmarked against experimental pilot plant data and models from independent research groups.

The validated steady-state model was used to determine a set of optimal operation parameters for post-combustion CO_2 capture using PZ. The results were created in Aspen Plus using the hybrid CAPCO₂ rate-based user model. This model considers slurry formation in the calculation of CO_2 mass transfer rate. According to the results, the capture process needs to be operated up to 14 % above the minimum achievable heat duty to avoid clogging from solid formation. 5 molal PZ offers the most promising trade-off between energy efficiency and solid-free operation with a specific reboiler duty of 3.22 GJ/t at 0.34 lean loading.

Furthermore, the project presents a dynamic rate-based model for CO_2 absorption and desorption using MEA and PZ as solvent. This dynamic model is an extension of the steady-state model as it uses the same thermodynamic, mass transfer, kinetic, and physical property modules. These modules are implemented in Fortran and interfaced with the dynamic model which is implemented in Matlab. The developed model was used to investigate the transient behavior of a post-combustion plant using MEA and PZ. Moreover, a proportional-integral control structure was developed to investigate the controllability of the PZ base post-combustion plant compared to the MEA plant. The results suggest that PZ may be a better solvent than MEA as it can accommodate disturbances with less variability in the manipulated variables. However, control design alternatives and/or model based control structures should be developed to reduce the long settling time of the PZ plant compared to the MEA plant.



Process flow diagram for acid gas recovery from a flue gas by amine absorption.

Enzymes in Enhanced Oil Recovery

Alsu Khusainova, PhD.

Full title:
"Enhanced Oil Recovery with Application of Enzymes"

Supervisors:
Alexander Shapiro, John Woodley

The project was funded by Innovation Fund Denmark, Novozymes, Maersk Oil, and DONG Energy as part of the BioRec project.

Direct link to this PhD thesis

Both laboratory experiments and some field tests have indicated that enzymes can be effective in Enhanced Oil Recovery (EOR). However, these studies have typically used commercial enzyme products composed of enzymes, surfactant and stabilizers, thus making it difficult to establish the exact mechanism behind the observed increase in oil recovery. The project focuses on the pure effect of the enzymes, and especially the relevance of enzyme EOR for Danish North Sea reservoirs.

Why would enzymes increase oil recovery? In the literature, four possible mechanisms have been suggested: wettability improvement of the rock surface; formation of emulsions; reduction of oil viscosity; and finally removal of high molecular weight paraffins.

By initial screening tests, lipases/esterases were identified as the most promising for further studies. This group of enzymes demonstrated strong ability to detach oil from the calcite surface. Here, wettability improvement due to protein adsorption onto the minerals was proposed as the main mechanism for enzymatic EOR. It was also proved that the enzyme molecules caused a change of the wetting state of calcite.

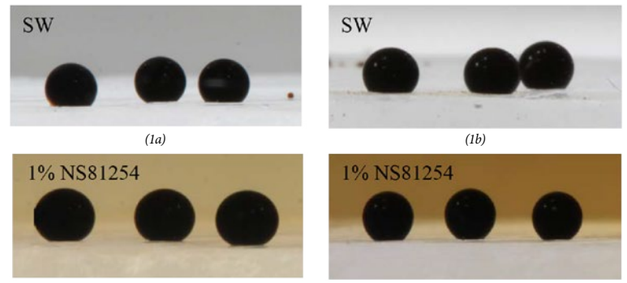
However, it would seem possible that this mechanism of enzymatic action could be limited under actual reservoir conditions, as protein molecules could become retained in the porous media. To verify this hypothesis, adsorption behavior of enzymes/proteins on the reservoir rocks was studied by application of static adhesion tests and adsorption experiments on powders, as well as dynamic flow-through experiments. It was established that enzymes are indeed significantly lost during transport in the porous media due to irreversible adsorption. The adsorption capacity of carbonate material was found to be much higher compared to sandstone. Various methods such as change of ionic strength and pH of the enzyme solution and displacing fluid were applied in attempts to desorb attached protein molecules, but without success.

Further, a second possible mechanism was studied, namely formation of enzyme-stabilized emulsions. Again, lipases/esterases were most promising, forming relatively stable emulsions with rather small drops. Incubation of the oil-[enzyme + sea water] system was found to be important for stability of the emulsions. Combined application of enzymes and solid particles was an alternative way to increase stability.

Other tests revealed additional problems that can rise in enzymatic EOR. Interaction of the enzyme solution with the crude oil can induce gelation/emulsification of the propylene glycol, which is the main component of the enzyme product stabilizers. Moreover, when purified enzyme containing almost no stabilizers was used, a highly viscous oil-in-water emulsion was formed.

Finally, two enzymes – lipase and amylase – were tested in flooding experiments under conditions similar to petroleum reservoirs. Application of the enzymes in sandstone core samples increased the ultimate oil production by 0.23 – 1.69 % relative to original oil in place. Wettability change was confirmed to be the main EOR mechanism, while emulsification plays a less significant role. In chalk, no increase in oil recovery was observed.

Overall, enzymes seem to possess a modest potential for EOR applications at least in sandstone and chalk reservoirs containing light crude oils. An alternative technique that will shift the adsorption balance towards reversible adsorption should be established in order to make enzymatic EOR effective and economically feasible.



(1a) *(1b)* *(2a)* *(2b)*

Effect of buoyancy on shape of the oil drops: 1a and 2a – shapes of the drops placed on the bottom surface of the mineral in presence of SW and 1% NS81254 sample, respectively; 1b and 2b – shapes of the drops placed on the top surface of the mineral in presence of SW and 1% NS81254 sample, respectively. Pictures in Figures 1a and 2a are turned upside down for easier comparison with Figures 1b and 2b.

Thermodynamic Modeling of CO_2 Mixtures

Martin Gamél Bjørner, PhD.
Currently with
EMCO Controls

Full title:
"Thermodynamic Modeling of CO_2 Mixtures"

Supervisor:
Georgios Kontogeorgis

The project was funded by the Danish Council for Independent Research / Technology and Production Sciences as part of the project CO_2 Hydrates – Challenges and Possibilities.

Direct link to this PhD thesis

Mixtures containing carbon dioxide occur in carbon capture and storage (CCS) but also in several other industrial processes. Prediction of the thermodynamic properties and phase equilibria of these mixtures is challenging. In the project, an extended version of an existing thermodynamic model is developed for the purpose.

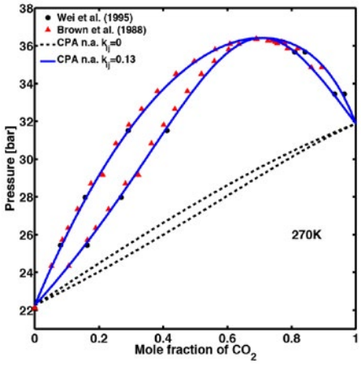
Reduction of CO_2 emissions by CCS is generally recognized as an important element in climate protection. Further, CCS can be combined with oil and gas production, if the captured CO_2 is used for enhanced oil recovery. In CCS, a CO_2 rich mixture is captured from an emission source - such as a power or cement plant - and transported to a storage point and ultimately stored underground. CCS requires knowledge of various thermodynamic properties as well as the phase behavior of mixtures containing CO_2 and hydrocarbons, water and/or other fluids such as alcohols and glycols.

Similar knowledge is necessary in other industrial processes with mixtures containing CO_2. An example is supercritical extractions, where CO_2 is used as a solvent.

CO_2 has a large quadrupole moment, i.e. a concentration of charges at four separate points in the molecule, which results in directional interactions. Classical cubic equations of state such as the SRK (Soave-Redlich-Kwong) do not take quadrupolar interactions into account. Even a modern equation of state such as the SAFT (Statistical Association Fluid Theory) only considers dispersive forces for CO_2.

In the project, the CPA (Cubic Plus Association) equation of state was extended to include quadrupole interactions. The new quadrupolar CPA – the qCPA – can be used with the experimental value of the quadrupole moment and with or without introducing an additional pure compound parameter. In the absence of quadrupolar compounds qCPA reduces to CPA, which itself reduces to SRK in the absence of association.

The new qCPA was evaluated for its ability to predict the thermodynamic properties of pure CO_2. The predictions were satisfactory. However, similar predictions were achieved by other CPA approaches. The model was subsequently evaluated for its ability to predict and correlate the binary VLE and LLE of mixtures containing CO_2 and n-alkanes, water, alcohols, or quadrupolar compounds. For these binary mixtures, qCPA appeared to offer systematically improved predictions and correlations as compared to the cases where quadrupolar interactions were ignored. The improvements were particularly pronounced for mixtures of CO_2 and hydrocarbons where the model is almost fully predictive.



Prediction (kij = 0) and correlation (kij = 0:13) of the CO_2 + ethane VLE at T=270 K using the CPA EoS with CO_2 modeled as an inert. Experimental data from [66, 67].

Finally, qCPA was evaluated for its ability to predict the phase equilibria of multi-component mixtures containing CO_2 and n-alkanes, water, and/or alcohols. A single binary interaction parameter was employed in qCPA for most binary combinations. Both qCPA and the best CPA approaches typically performed satisfactorily, but qCPA used few adjustable parameters to achieve the predictions.

In conclusion, it has been demonstrated that qCPA is a promising model which, compared to CPA, systematically improves the predictions of the experimentally determined phase equilibria between binary and ternary mixtures containing CO_2 and other non-quadrupolar compounds.

Oil-water Interactions during Smart Water Flooding

Artem Alexeev, PhD.
Currently Postdoc at CERE

Full title:
"Modeling of Salinity Effects on Water Flooding of Petroleum Reservoirs"

Supervisors:
Alexander Shapiro, Kaj Thomsen

The project was funded by DONG Energy, Maersk Oil, and the Danish EUDP program (for development and demonstration of energy technology) under the Danish Energy Agency, and by the Danish research councils.

Direct link to this PhD thesis

Water flooding of petroleum reservoirs was introduced more than a century ago. Injection of water with a composition deliberately altered to improve recovery is named "smart water flooding". Extensive studies over the last 20 years have clearly demonstrated an additional effect over standard flooding. However, no agreement has been reached on the determining mechanism. The project aims to advance understanding of this issue.

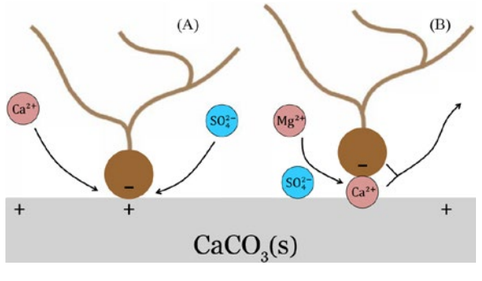
In the project, a generic model for the reactive transport in porous media was set up, and several phenomena such as mineral dissolution, adsorption of potential determining ions in carbonate rocks, and mechanisms that influence mobilization of the trapped oil and its transport were considered.

Initially, the formation water will be in equilibrium with the reservoir rock. When brine with a composition different from the formation water is introduced, the equilibrium is disturbed, resulting in dissolution of minerals from the rock.

In the project it was found, that the rate of dissolution has a significant influence on the evolution of the rock properties. At low reaction rates, dissolution occurs across the entire region between the injection and production sites resulting in heterogeneous porosity and permeability fields. Fast dissolution resembles formation of wormholes with a significant change in porosity and permeability close to the injection site.

The oil trapped in swept zones after conventional flooding is present as disconnected drops, or oil ganglia. Both oil and water can be present in a single pore body and interact during the flow. It was found, that presence of water on the rock surface and in the corner filaments of pore bodies result in a larger velocity of the viscous flow of the oil phase due to the increased area of the moving oil-water interface. Moreover, the flow of oil may be induced solely by the action of viscous forces at the oil-water interface, which appears to be a new mechanism for the transport of oil ganglia in porous media.

Further, a macroscopic model of displacement accounting for the effects of oil ganglia was developed. Numerical modeling showed that production of oil ganglia may continue for a long time of injection of around 10 to 20 PVI (Pore Volumes Injected).



Schematic model of the suggested mechanism for the wettability alteration induced by seawater. (A) Proposed mechanism when Ca_{2+} and SO_{42-} are the active species. (B) Proposed mechanism when Mg_{2+} and SO_{42-} are the active species. Reproduced after Zhang et al. [5]

Unlike the conventional models of chemical flooding, where the mobilized oil bank travels ahead of the concentration front, the oil ganglia model predicts that the mobilized oil is produced after the active species reach the effluent.

Alteration of the electrostatic potential is a possible mechanism for mobilization of the residual oil in carbonates. Reduction of the surface charge due to adsorption of the potential determining ions results in a decrease in oil affinity towards the rock surface. To investigate how the composition of the injected brine affects the equilibrium surface composition, a mathematical model was established. The model takes adsorption of the potential determining ions – calcium, magnesium, and sulfate – into account. Parameters for the model were estimated from experimental data on the produced brine composition and flow-through experiments. The computations suggest no evidence of usually assumed stronger adsorption of magnesium ion compared to calcium at high temperatures.

Computations of the equilibrium surface composition demonstrate a correlation between the concentration of the adsorbed sulfate and the ultimate recovery observed in the experiments indicating that a more negatively charged surface of chalk could be a factor that affects the recovery efficiency without wettability modification.

Professor Georgios Kontogeorgis, Chairman of CERE speaking at Thermodynamics 2015, Copenhagen, Denmark in September.

Conference Contributions

JANUARY

32nd Nordic Geological Winter meeting, Helsinki, Finland, 13–15 January, 2016

I.L. Fabricius, "Burial stress and burial strain", 32nd Nordic Geological Winter meeting, Helsinki, Finland, 13–15 January, 2016 (oral – book of abstracts 258-259)

L. Paci, L. Pasquinelli and I.L. Fabricius, "Geological 3D modelling of claistic rocks. A case study from Stenlille Structure, Denmark", 32nd Nordic Geological Winter Meeting, Helsinki, Finland, 13–15 January, 2016 (oral, book of abstracts, 309-310)

L. Pasquinelli, "Porosity, permeability, thermal properties of clastic rocks. A case study in Stenlille structure, Denmark", 32nd Nordic Geological Winter meeting, Helsinki, Finland, 13–15 January, 2016 (oral, book of abstracts, 305-306)

Ben Gurion University, Beer Sheva, Israel, 25 January, 2016

I.L. Fabricius, "Burial stress and elastic strain of carbonate rocks", Ben Gurion University, Beer Sheva, Israel, 25 January, 2016 (invited lecture)

FEBRUARY

UTCCS-3, The Third University of Texas Conference on Carbon Capture and Storage, Austin, Texas, USA, 17–19 February, 2016

P.L. Fosbøl, A. Gladis, J. Glibstrup, and J. Gaspar, "Enzymes in CO_2 capture", UTCCS-3, The Third University of Texas Conference on Carbon Capture and Storage, Austin, Texas, USA, 17–19 February, 2016 (oral)

P.L. Fosbøl, "Measurement of properties and pilot testing", UTCCS-3, The Third University of Texas Conference on Carbon Capture and Storage, Austin, Texas, USA, 17–19 February, 2016

APRIL

SPE Improved Oil Recovery Conference, Tulsa, Oklahoma, USA, 11–13 April, 2016

D. Paterson, W. Yan, M.L. Michelsen, and E.H. Stenby, "Robust and efficient isenthalpic flash algorithms for thermal recovery of heavy oil", SPE Improved Oil Recovery Conference, Tulsa, Oklahoma, USA, 11–13 April, 2016 (oral + conference paper)

SPE Bergen One Day Seminar, Bergen, Norway, 20 April, 2016

M. Ahkami, K.H. Chakravary, I. Xiarchos, K. Thomsen, and P.L. Fosbøl, "Determining optimum aging time using novel core flooding equipment", SPE Bergen One Day Seminar, Bergen, Norway, 20 April, 2015 (oral)

IOR Norway 2016, Stavanger, Norway, 25–27 April, 2016

T. Livada, A. Nermoen, R.I. Korsnes, and I.L. Fabricius, "Effects of temperature cycles on mechanical parameters of chalk." IOR Norway 2016, Stavanger, Norway, 25–27 April, 2016 (poster)

MAY

EFCE Working Party on Fluid Separations 58th Technical Meeting, Copenhagen, Denmark, 12 May, 2016

P.L. Fosbøl, "Measurement of properties and pilot testing", EFCE Working Party on Fluid Separations 58th Technical Meeting, Copenhagen, Denmark, 12 May, 2016 (oral)

14th International Conference on Properties and Phase Equilibria for Product and Process Design, Porto, Portugal, 22–26 May, 2016

A. Arya, Nicolas von Solms, and G. Kontogeorgis, "Modeling of asphaltene precipitation using CPA & PC-SAFT Equations of State", 14th International Conference on Properties and Phase Equilibria for Product and Process Design, Porto, Portugal, 22–26 May, 2016 (poster)

G. Kontogeorgis, "20 years with the CPA equation of state", 14th International Conference on Properties and Phase Equilibria for Product and Process Design, Porto, Portugal, 22–26 May, 2016 (oral)

A. Schlaikjer, K. Thomsen, and G. Kontogeorgis, "Simultaneous description of activity coefficients and solubility with electrolyte CPA", 14th International Conference on Properties and Phase Equilibria for Product and Process Design, Porto, Portugal, 22–26 May, 2016 (poster)

C. Tsanas, W. Yan, and E.H. Stenby, "A new algorithm for simultaneous chemical and phase equilibrium calculation", 14th International Conference on Properties and Phase Equilibria for Product and Process Design, Porto, Portugal, 22–26 May, 2016 (poster)

A.P.C.M. Vinhal, "Critical point prediction using CPA for pure and multicomponent systems", 14th International Conference on Properties and Phase Equilibria for Product and Process Design, Porto, Portugal, 22–26 May, 2016 (poster)

78th EAGE Conference & Exhibition 2016, Vienna, Austria, 30 May–2 June, 2016

K. Katika, M, Saidian, and I.L. Fabricius, "Wettability of chalk and argillaceous sandstones assessed from T1/T2 ratio." Paper presented at 78th EAGE Conference & Exhibition 2016, Vienna, Austria, 30 Maj–2 June, 2016 (oral)

JUNE

78th EAGE Conference & Exhibition including SPE EUROPEC, Vienna, Austria, 30 May–2 June, 2016

F. Varzandeh, W. Yan, and E. H. Stenby, "General Approach to Characterize Reservoir Fluids Using a Large PVT Database", 78th EAGE Conference & Exhibition including SPE EUROPEC, Vienna, Austria, 30 May–2 June, 2016 (oral)

European Congress on Computational Methods in Applied Science and Engineering, ECCOMAS Congress 2016, Crete Island, Greece, 5–10 June, 2016

C.S. Hemmingsen, J.H. Walther, "Multiphase Flow in Porous Media Using CFD", European Congress on Computational Methods in Applied Science and Engineering, ECCOMAS Congress 2016, Crete Island, Greece, 5–10 June, 2016 (oral)

DYCOPS-CAB 2016, Trondheim, Norway, 6–8 June, 2016

J. Gaspar, L. Ricardez-Sandoval, J.B. Jørgensen, and P.L. Fosbøl, "Dynamic simulation and analysis of a pilot-scale CO2 post-combustion capture unit using piperazine and MEA", DYCOPS-CAB 2016, Trondheim, Norway, 6–8 June, 2016 (oral)

14th European Powder Diffraction Conference (EPDIC 2016), Bari, Italy, 12–15 June, 2016

K. Ståhl, R. Neerup, and P.L. Fosbøl, "CO_2 capture. Two new structures in the 2-amino-2-methyl-1propanol (AMP) – water – CO_2 system", 14th European Powder Diffraction Conference (EPDIC 2016), Bari, Italy, 12–15 June, 2016 (poster)

The 17th International Conference on Petroleum Phase Behavior and Fouling, Elsinore, Denmark, 19–23 June, 2016

S. Almeida, L.G. Martos, J.B. Costa, R. Lundsgaard, G. Kontogeorgis, J. Sonne, C. Wang, A. Rubin, and N.V. Solms, "Thermodynamics and transport of gases in polymer liners for subsea applications", The 17th International Conference on Petroleum Phase Behavior and Fouling, Elsinore, Denmark, 19–23 June, 2016

A. Arya, Nicolas von Solms, and G. Kontogeorgis, "Modeling of asphaltene onset precipitation conditions using the CPA & PC-SAFT Equations of State", The 17th International Conference on Petroleum Phase Behavior and Fouling, Elsinore, Denmark, 19–23 June, 2016 (oral)

X. Liu, W. Yan, F. Pettersson, P. Svensson, E.H. Stenby, and E. Thormann, "QCM-D study of adsorption and desorption of crude oil on and from silica and calcium carbonate surfaces", The 17th International Conference on Petroleum Phase Behavior and Fouling, Elsinore, Denmark, 19–23 June, 2016 (oral)

L. Mu, and N. von Solms, "Methane production and carbon capture by hydrate swapping", The 17th International Conference on Petroleum Phase Behavior and Fouling, Elsinore, Denmark, 19–23 June, 2016 (poster)

European Control Conference 2016, Aalborg, Denmark, 29 June–1 July, 2016

J.B. Jørgensen, L.E. Sokoler, L. Standardi, R. Halvgaard, T.G. Hovgaard, G. Frison, N.K. Poulsen, and H. madsen, "Economic MPC for a linear stochastic system of energy units", European Control Conference 2016, Aalborg, Denmark, 29 June–1 July, 2016 (oral)

JULY

ISSP 2016 17th International Symposium on Solubility Phenomena and Related Equilibrium Processes, Geneva, Switzerland, 24–29 July, 2016

D.C. Figueroa, P.L. Fosbøl, and K. Thomsen, "Solubility measurements and modeling of zinc, lead and iron sulfides at high temperatures and high pressures", ISSP 2016 17th International Symposium on Solubility Phenomena and Related Equilibrium Processes, Geneva, Switzerland, 24–29 July, 2016 (oral)

Kaj Thomsen, "Thermodynamic modeling of the solubility of silica", International Symposium on Solubility Phenomena and Related Equilibrium Processes (ISSP), Geneva, Switzerland, 24–29 July, 2016 (oral)

AUGUST

International Symposium of the Society of Core Analysts, Snowmass, Colorado, USA, 21–26 August 2016

T. Livada, A. Nermoen, R.I. Korsnes, and I.L. Fabricius, "To what degree thermal cycles affect chalk strength", International Symposium of the Society of Core Analysts, Snowmass, Colorado, USA, 21–26 August, 2016 (poster, SCA2016-087, 1-7)

CHISA conference, Prague, Czech Republic, 27–31 August, 2016

Arne Gladis, Maria T.Gundersen, Philip .L. Fosbøl, John M. Woodley, and Nicolas von Solms, "How to use carbonic anhydrase enzymes in carbon capture technology"; CHISA conference, Prague, Czech Republic, 27–31 August, 2016 (oral)

15th European Conference on the Mathematics of Oil Recovery (ECMOR XV), Amsterdam, The Netherlands, 29 August–1 September, 2016

D. Paterson, W. Yan, M.L. Michelsen, and E.H. Stenby, "Isenthalpic flash for thermal recovery", 15th European Conference on the Mathematics of Oil Recovery (ECMOR XV), Amsterdam, The Netherlands, 29 August–1 September, 2016 (oral + conference paper)

D. Sandoval, "Model comparison for high-pressure adsorption in shale and its influence on phase equilibria", 15th European Conference on the Mathematics of Oil Recovery (ECMOR XV), Amsterdam, The Netherlands, 29 August–1 September, 2016 (oral + conference paper)

SEPTEMBER

Reservoir Management Optimization Workshop, TNO, Utrecht, The Netherlands, 2 September, 2016

J.B. Jørgensen, "Risk minimization in life-cycle oil production optimization", Reservoir Management Optimization Workshop, TNO, Utrecht, The Netherlands, 2 September, 2016 (oral)

Magnetic Resonance in Porous Media Conference (MRPM13), Bologna, Italy, 4–8th September, 2016

K. Katika, H. Fordsmand, and I.L. Fabricius, "Low field NMR surface relaxivity studies of chalk and argillaceous sandstones", Magnetic Resonance in Porous Media Conference (MRPM13), Bologna, Italy, 4–8 September, 2016 (oral, Book of Abstracts, O28)

10th International Geostatistics Congress, Valencia, Spain, 5–9 September, 2016

S. Khoshkholgh, A. Zunino, T.M. Hansen, and K. Mosegaard, "Coupled multi-scale well and surface seismic data inversion using wavelet decomposition", 10th International Geostatistics Congress, Valencia, Spain, 5–9 September, 2016

IEA-EOR 2016 37th Annual Workshop & Symposium, Paris, France, 18–22 September, 2016

H. Baghooee, and A.A. Shapiro, "Mechanics of the waterflooding accounting for motion of the water-oil interface", IEA-EOR 2016 37th Annual Workshop & Symposium, Paris, France, 18–22 September, 2016 (oral)

I. Nesterov, A. Alexxev, S.M. Nielsen, A.A. Shapiro, and E.H. Stenby, "Microbial enhanced oil recovery. Computational study of selective plugging in the porous media", IEA-EOR 2016 37th Annual Workshop & Symposium, Paris, France, 18–22 September, 2016 (oral)

D. Paterson, W. Yan, M.L. Michelsen, and E.H. Stenby, "Multiphase isenthalpic flash for thermal recovery", IEA-EOR 2016 37th Annual Workshop & Symposium, Paris, France, 18–22 September, 2016 (oral)

D. Sandoval, G. Lubelli, W. Yan, M.L. Michelsen, and E.H. Stenby, "Effects of capillary pressure and adsorption on phase equilibrium in porous media", IEA-EOR 2016 37th Annual Workshop & Symposium, Paris, France, 18–22 September, 2016 (oral)

Core Workshop, Norweigian Petroleum Directorate, 20 September, 2016

I.L. Fabricius, "Ekofisk formation in South Arne Field", Core Workshop, Norweigian Petroleum Directorate, 20 September, 2016 (invited lecture)

OCTOBER

The 11th Asian Thermophysical Properties Conference, Yokohama, Japan, 2–6 October, 2016

T. Regueira, E.H. Stenby and W. Yan, "Phase Equilibrium and volumetric properties of asymmetric hydrocarbon mixtures at high pressures and high temperatures", The 11th Asian Thermophysical Properties Conference, Yokohama, Japan, 2–6 October, 2016 (oral)

First Nordic Phosphorus Conference, Phosphorus a limited resource – Closing the Loop, 27–28 October, 2016

K. Thomsen, "Struvite-K, sustainable recovery of pure phosphate from sewage sludge and biomass ash", First Nordic Phosphorus Conference, Phosphorus a limited resource - Closing the Loop, 27–28 October, 2016 (poster)

NOVEMBER

Chemical Engineering School of the National Polytechnic Institute of Mexico, ESIQIE, "Sustainable Engineering in the transformation of the natural resources", Mexico City, Mexico, 7–12 November, 2016

G. Kontogeorgis, "Some applications of thermodynamics for a sustainable chemical engineering with emphasis on energy", Chemical Engineering School of the National Polytechnic Institute of Mexico, ESIQIE, "Sustainable Engineering in the transformation of the natural resources", Mexico City, Mexico, 7–12 November, 2016 (invited lecture)

AIChE Annual Meeting, San Francisco, USA, 13–18 November, 2016

A. Gladis, M.T. Gundersen, P.L. Fosbøl, J.M. Woodley, and N.V. Solms; "Carbonic anhydrase enhanced carbon capture: Kinetic measurements and pilot plant trials", AIChE Annual Meeting, San Francisco, USA, 13–18 November, 2016 (oral)

13th International Conference on Greenhouse Gas Control Technologies (GHTT-13), Lausanne, Switzerland, 14–18 November, 2016

M.W. Arshad, P.L. Fosbøl, N.V. Solms, and K. Thomsen, "CO_2 Capture with liquid-liquid phase change solvents: A thermodynamic study", 13th International Conference on Greenhouse Gas Control Technologies (GHTT-13), Lausanne, Switzerland, 14–18 November, 2016 (oral)

D. Bonalumi, Stefano Lillia, Gianluca Valenti, P.L. Fosbøl, and K. Thomsen, "Kinetic study of a layout for the carbon capture with aqueous ammonia without salt precipitation", 13th International Conference on Greenhouse Gas Control Technologies (GHTT-13), Lausanne, Switzerland, 14–18 November, 2016 (poster)

A. Gladis, M.T. Gundersen, K. Thomsen, P.L. Fosbøl, J.M. Woodley, and N. von Solms, "Comparison of the kinetic promoters piperazine and carbonic anhydrase for CO_2 absorption", 13th International Conference on Greenhouse Gas Control Technologies (GHTT-13), Lausanne, Switzerland, 14–18 November, 2016 (oral)

A. Gladis, N. Lomholdt, P.L Fosbøl, J. Woodley, and N. von Solms, "Pilot absorption experiments with carbonic anhydrase enhanced MDEA", 13th International Conference on Greenhouse Gas Control Technologies (GHTT-13), Lausanne, Switzerland, 14–18 November, 2016 (poster)

M.T. Gundersen, A. Gladis, P.L. Fosbøl, N. von Solms, and J.M. Woodley, "Operating windows for enzyme enhanced PCCC", 13th International Conference on Greenhouse Gas Control Technologies (GHTT-13), Lausanne, Switzerland, 14–18 November, 2016 (poster)

J. Gaspar, A. Gladis, J. Woodley, K. Thomsen, N. von Solms, and P.L. Fosbøl, "Rate-based modelling and validation of a pilot absorber using MDEA enhanced with carbonic anhydrase (CA)", 13th International Conference on Greenhouse Gas Control Technologies (GHTT-13), Lausanne, Switzerland, 14–18 November, 2016 (poster)

J. Gaspar, P.L. Fosbøl, "Design, economics, and parameter uncertainty in dynamic operation of post-combustion CO_2 capture using piperazine (PZ) and MEA solvents", 13th International Conference on Greenhouse Gas Control Technologies (GHTT-13), Lausanne, Switzerland, 14–18 November, 2016 (oral)

P.L. Fosbøl, J. Gaspar, J. Glibstrup, A. Gladis, K.M. Diaz, K. Thomsen, and N. von Solms, "Design and simulation of rate-based CO2 capture processes using carbonic anhydrase (CA) applied to biogas, natural gas and coal cases", 13th International Conference on Greenhouse Gas Control Technologies (GHTT-13), Lausanne, Switzerland, 14–18 November, 2016 (poster)

DHRTC Technology Conference, Helsingør, Denmark, 16–17 November, 2016

M.W. Arshad, P.L. Fosbøl, A. Shapiro, and K. Thomsen, "Effect of fines particle size on emulsion formation in Smart Water EOR", DHRTC Technology Conference, Helsingør, Denmark, 16–17 November, 2016 (poster)

S. Gupta, "Feasibility and existing knowledge on test rigs for determining under deposit corrosion (UDC) mechanisms", DHRTC Technology Conference, Helsingør, Denmark, 16–17 November, 2016 (poster)

J.B. Jørgensen, "Life-cycle oil production optimization using proper tisk-measures and closed-loop reservoir management", DHRTC Technology Conference, Helsingør, Denmark, 16–17 November, 2016 (oral)

L.T. Pinto, "Overview of geo-mechanical properties from Dand neighbouring fields", DHRTC Technology Conference, Helsingør, Denmark, 16–17 November, 2016 (oral)

K. Thomsen, "Thermodynamic modeling of Smartwater", DHRTC Technology Conference, Helsingør, Denmark, 16–17 November, 2016 (oral)

F. Varzandeh, E. H. Stenby, W. Yan, "Evaluation of the Impact of Compositional Characterization of Reservoir Fluids on Modeling", DHRTC Technology Conference, Helsingør, Denmark, 16–17 November, 2016 (Poster)

Master Theses 2016

Maha Mohamad Abou El Zalaf
"Thermal maturation and elasticity of oil shale from Shephela Basin"

Thordis Bjørnsdottir
"Assessment of mud weight in deep wells"

Tummas Pauli Hanusarson
"Rate-dependent Compaction of Chalk and Porefluid Influence"

Georgios Aloupis
"Modeling of Thermodynamics of Hydrate Inhibitor Systems"

Christos Panagiotis Chatziagapiou
"Joule-Thomson coefficeients of hydrocarbon mixtures at high pressures"

Jiasheng Hao
"Experimental study of enhanced oil recovery by application of advanced chemicals"

Mehrshad Ashrafi
"PVT study of hydrocarbon mixtures at high pressure and high temperature conditions"

Kevin Julio Milla Diaz
"Simulation of enzyme-based biogas upgrading"

Ehab Hendi
"Quantitative mud gas interpretation"

Hadise Baghohee
"Propagation of the liquid-liquid interface in a two-phase flow in a porous medium"

Gianni Ferrero
"Development of 3D Graphene structures for oil-water separation"

Aqeel Hussain
"Petrophysical interpretation, Kraka field"

Finlay Gordon Mackenzie Bertram
"Simulation of Low Salinity Water Flooding"

Joachim Christian Franch
"Cyclic triaxial testing of chalk"

Pawel Igor Janus
"Anisotropy of plastic clays"

Christian Frausing Brams
"A study on multiscale techniques for reservoir simulation"

Nipon Garg
"Fines formation during CO_2 low salinity WAG (CO_2LSWAG) EOR"

ILias Kravvaritis
"Wellbore stability and mud weight window of geothermal wells"

Thomas Bruun Berthelsen
"Uncertainty quantification, filtering and prediction for oil reservoir operations"

George Minta Gyimah
"Investigation of end-effects on UCS specimens"

Yiqun Liu
"PVT study of model reservoir fluids at HPHT conditions"

Gianluca Lubelli
"Phase Equilibrium Calculation in the Presence of Capillary Pressure"

Ishan Shukla
"Adsorption of mixtures in microporous media"

Konstantinos Lymperis
"Analysis of core flooding experiments: The role of fines in Enhanced Oil Recovery"

Hiba Sobeir
"Wellbore statbility and mud weight window of geothermal wells"

Adam Andrzej Marczynski
"Coupling of stiffness and thermal properties for sedimentary rocks"

Yuanmei Song
"Promotion of methane hydrate formation by adding trace gases"

Søren Mortensen
"Further development of the electrolyte equation of state for electrolyte systems"

Márton László Szanyi
"Near-wellbore multiphase flow modeling with computational fluid dynamics"

Robin Pronk
"Experimental study of clay fines migration as a consequence of low-salinity water injection"

Kasper Torbensen
"Proactive well workover & maintenance model"

Alejandro Rodriguez Pupo
"Thermodynamic modeling of scale formation in brines from HP/HT reservoirs"

Edgar Luis Camacho Vergara
"Modelling gas hydrates with improved Langmuir adsorption constants"

Maciej Rzuchowski
"Petrophysical interpretation of logs from organic rich chalks"

Ahmad Adyarso Wibowo
"PVT study of model reservoir fluids at HPHT conditions"

Publications

Publications submitted in previous years and published in 2016

CERE 1503

"Hydrate Equilibrium Data for the CO_2-N_2 System with the use of Tetra-n-butylammonium Bromide (TBAB), Cyclopentane (CP) and their Mixture"

Fragkiskos Tzirakis, Paolo Stringari, Nicolas von Solms, Christophe Coquelet, and Georgios M. Kontogeorgis (Fluid Phase Equilibria, 408 (2016) 240-247)

CERE 1505

"A Comment on Water´s Structure using Monomer Fraction Data and Theories"

Xiaodong Liang, Bjørn Maribo-Mogensen, Ioannis Tsivintzelis, and Georgios M. Kontogeorgis (Fluid Phase Equilibria, 407 (2016) 2-6)

CERE 1510

"Modelling Phase Equilibria for Acid Gas Mixtures using the CPA Equation of State. Part VI. Multicomponent Mixtures with Glycols Relevant to Oil & Gas and Liquid or Supercritical CO_2 Transport Applications"

Ioannis Tsivintzelis, and Georgios M. Kontogeorgis (Journal of Chemical Thermodynamics, 93 (2016) 305-319)

CERE 1511

"A Collocation Method for Surface Tension Calculation with the Density Gradient Theory"

Peter Mahler Larsen, Bjørn Maribo-Mogensen, and Georgios M. Kontogeorgis (Fluid Phase Equilibria, 408 (2016) 170-179)

CERE 1517

"Modeling Derivative Properties and Binary Mixtures with CO_2 using the CPA and the Quadrupolar CPA Equations of State"

Martin Gamél Bjørner, and Georgios M. Kontogeorgis (Fluid Phase Equilibria, 408 (2016) 151-169)

CERE 1523

"Mechanics of the Separating Surface for a Two-phase Co-current Flot in a Porous Medium"

Alexander A. Shapiro (Transport in Porous Media, 112 (2016) 489-517)

CERE 1524

"Modeling of Phase Equilibrium of North Sea Oils with Water and MEG"

Michael Frost, Georgios M. Kontogeorgis, Nicolas von Solms, and Even Solbraa (Fluid Phase Equilibria, 424 (2016) 79-89)

CERE 1525

"Investigation of the Gas Injection Effect on Asphaltene Onset Precipitation Using the Cubic-Plus-Association Equiation of State"

Alay Arya, Nicolas von Solms, and Georgios M. Kontogeorgis (Energy & Fuels, 30 (2016) 3560-3574)

CERE 1527 *"Microbial Enhanced Oil Recovery – A Modeling Study of the Potential of Spore-forming Bacteria"*

S. M. Nielsen, I. Nesterov, and A. A. Shapiro (Computational Geosciences, 20 (2016) 567-580)

CERE 1530 *"The Phase Envelope of Multicomponent Mixtures in the Presence of a Capillary Pressure Difference"*

Diego Sandoval, Wei Yan, Michael L. Michelsen, Erling H. Stenby (Ind. Eng. Chem. Res., 55 (2016) 6530-6538)

CERE 1532 *"Uncertainty Analysis of the CPA and a Quadrupolar CPA Equation of State – With emphasis on CO_2"*

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

CERE 1538 *"Time-Explicit Methods for Joint Economical and Geological Risk Mitigation in Production Optimization"*

Lasse H. Christiansen, Andrea Capolei, and John Bagterp Jørgensen (Journal of Petroleum Science and Engineering, 146 (2016) 158-169)

CERE 1541 *"Dynamic Operation and Simulation of Post-Combustion CO_2 Capture"*

Jozsef Gaspar, Arne Gladis, John Bagterp Jørgensen, Kaj Thomsen, Nicolas von Solms, and Philip Loldrup Fosbøl (Energy Procedia, 86 (2016) 205-214)

CERE 1543 *"Multivariable Optimization of the Piperazine CO_2 Post-Combustion Capture Process"*

Jozsef Gaspar, Nicolas von Solms, Kaj Thomsen, and Philip Loldrup Fosbøl (Energy Procedia, 86 (2016) 229-238)

CERE 1544 *"Pitfalls of using the Geometric-mean Combining Rule in the Density Gradient Theory"*

Xiaodong Liang, Michael Locht Michelsen, and Georgios M. Kontogeorgis (Fluid Phase Equilibria, 415 (2016) 75-83)

CERE 1545 *"Modelling the Phase Equilibria of Multi-component Mixtures Containing CO2, Alkanes, Water and/or Alcohols using the Quadrupolar CPA Equation of State"*

Martin G. Bjørner, and Georgios M. Kontogeorgis (Molecular Physics, 114 (2016) 2641-2654)

CERE Publications submitted in 2016

CERE 1601 *"Solubility Modeling of the Binary Systems $Fe(NO_3)_3$-H_2O, $Co(NO_3)_2$-H_2O and the Ternary $Fe(NO_3)_3$-$Co(NO_3)_2$-H_2O with the Extended Universal Quasichemical (UNIQUAC) Model"*

Mouad Arrad, Mohammed Kaddami, Bahija El Goundali, and Kaj Thomsen (Journal of Solution Chemistry, 45 (2016) 534-545)

CERE 1602 *"Thermodynamic Modeling of Liquid-Liquid Phase Change Solvents for CO_2 Capture"*

Muhammad Waseem Arshad, Nicolas von Solms, and Kaj Thomsen (Greenhouse Gas Control, 53 (2016) 401-424)

CERE 1603 *"Application of Various Water Soluble Polymers in Gas Hydrate Inbibition"*

Muhammad Shahzad Kamal, Ibnelwaleed A. Hussein, Abdullah S. Sultan, and Nicolas von Solms (Renewable and Sustainable Energy Reviews, 60 (2016) 206-225

CERE 1605 *"Simulation and Multivariable Optimization of Post-Combustion Capture using Piperazine"*

Jozsef Gaspar, and Philip Loldrup Fosbøl (International Journal of Greenhouse Gas Control, 49 (2016) 227-238)

CERE 1610 *"Volumetric Behavior of Six Ionic Liquids from T=(278 to 398)K and up to 120MPa"*

Félix M. Gaciño, Teresa Muñiz Regueira, Alexander V. Bolotov, Artur Sharipov, Luis Lugo, María J.P. Fernández, and Josefa Fernández (Journal of Chemical Thermodynamics, 93 (2016) 24-33)

CERE 1611 *"Density and Phase Equilibrium of the Binary System Methane + n-decane under High Temperatures and Pressures"*

Teresa Regueira, Georgia Pantelide, Wei Yan, and Erling H. Stenby (Fluid Phase Equilibria, 428 (2016) 48-61)

CERE 1613 *"Modeling Systems Relevant to the Biodiesel Production Using the CPA Equation of State. Part 1. Pure compounds and binary systems"*

Ioannis Tsivintzelis, Shahid Ali, and Georgios M. Kontogeorgis (Fluid Phase Equilibria, 430 (2016) 75-92)

CERE 1614 *"Modeling Systems Relevant to the Biodiesel Production Using the CPA Equation of State. Part 1. Pure compounds and binary systems." Supplementary Material*

Ioannis Tsivintzelis, Shahid Ali, and Georgios M. Kontogeorgis (Fluid Phase Equilibria, 430 (2016) 75-92)

CERE 1616 *"Modeling of Asphaltene Onset Precipitation Conditions with Cubic Plus Association (CPA) and Perturbed Chain Statistical Associating Fluid Theory (PC-SAFT) Equation of States"*

Alay Arya, Xiaodong Liang, Nicolas von Solms, and Georgios Kontogeorgis (Energy & Fuels, 30 (2016) 6835-6852)

CERE 1618 *"A Density Gradient Theory Based Method for Surface Tension Calculations"*

Xiaodong Liang, Michael Locht Michelsen, and Georgios M. Kontogeorgis (Fluid Phase Equilibria, 428 (2016) 153-163)

CERE 1619 *"Release of Crude Oil from Silica and Calcium Carbonate Surfaces: On the Alternation of Surface and Molecular Forces by High- and Low-Salinity Aqueous Salt Solutions"*

Xiaoyan Liu, Wei Yan, Erling H. Stenby, and Esben Thormann (Energy & Fuels, 30 (2016) 3986-3993)

CERE 1620 *"Evaluation of CPA EoS (cubic-plus-association equation of state) for ternary, quaternary and multicomponent systems in the presence of mono-ethylene glycol (MEG))*

Fragkiskos Tzirakis, Eirini Karakatsani, and Georgios M. Kontogeorgis (Industrial & Engineering Chemistry Research, 55 (2016) 11371-11382)

CERE 1624 *"Unstructured Spectral Element Model for Dispersive and Novlinear Wave Propagation"*

Allan P. Ensig-Karup, Claes Eskilsson, Daniele Bigoni (In Proceedings of The 26th International Ocean and Polar Engineering Conference (ISOPE), 26 June – 2 July, 2016, Society of Petroleum Engineers, 2016 661-668 ISOPE-I-16-455)

CERE 1626 *"Predictive Screening of Ionic Liquids for Dissolving Cellulose and Experimentel Verification"*

Yan-Rong Liu, Kaj Thomsen, Yi Nie, Suo-Jiang Zhang, and Anne S. Meyer (Green Chemistry, 18 (2016) 6147-6398)

CERE 1628 *"A Layout for the Carbon Capture with Aqueous Ammonia without Salt Precipitation"*

Davide Bonalumi, Gianluca Valenti, Stefano Lillia, Philip L. Fosbøl, and Kaj Thomsen (Energy Procedia, 86 (2016) 134-143)

CERE 1629 *"Controllability and Flexibility Analysis of CO_2 Post-combustion Capture using Piperazine and MEA"*

Jozsef Gaspar, Luis Ricardez-Sandoval, John Bagterp Jørgensen, and Philip L. Fosbøl (International Journal of Greenhouse Gas Control, 51 (2016) 276-289)

CERE 1630 *"Determining Optimum Aging time using Novel Core Flooding Equipment"*

Mehrdad Ahkami, Krishna Hara Chakravarty, Ioannis Xiarchos, Kaj Thomsen, Philip L. Fosbøl (Proceedings of the 23rd International SPE Bergen One Day Seminar, Society of Petroleum Engineers, SPE-180054-MS (2016) 1-16)

CERE 1631 *"Hydrate Equilibrium Data for CO_2+N_2 System in the Presence of Tetra-n-butylammonium Fluoride (TBAF) and Mixture of TBAF and Cyclopentane (CP)*

Fragkiskos Tzirakis, Paolo Stringari, Christophe Coquelet, Nicolas von Solms, and Georgios Kontogeorgis (Journal of Chemical and Engineering Data, 61 (2016) 1007-1011)

CERE 1632 *"Irreversible Change of the Pore Structure of ZIF-8 in Carbon Dioxide Capture with Water Coexistence"*

Huang Liu, Ping Guo, Teresa Regueira Muñiz, Zhouhua Wang, Jianfen Du, and Guangjin Chen (Journal of Physical Chemistry C, 120 (2016) 13287-13294)

CERE 1637 *"Comparative analysis of experimental methods for quantification of small amounts of oil in water"*

Katika, K., Ahkami, M., Fosbøl, P.L., Halim, A.Y., Shapiro, A., Thomsen, K., Xiarchos, I. & Fabricius, I.L. (Journal of Petroleum Science and Engineering, 147 (2016) 459–467)

CERE 1638 *"New insight into the microtexture of chalks from NMR analysis"*

O. Faÿ, J. Soete, K. Katika, S. Galaup, B. Caline, F. Descamps, E. Lasseur, I.L. Fabricius, J. Saïag, R. Swennen, and S. Vandycke (Marine and Petroleum Geology, 75 (2016) 252-271)

CERE 1640 *"Optimizing integrated reference cases in the OCTAVIUS project"*

H.M. Kvamsdala, S. Ehlers, A. Kather, P. Khakharia, M. Nienoord, and P.L. Fosbøl (International Journal of Greenhouse Gas Control, 50 (2016)23-36)

CERE 1641 *"Low immediate scientific yield of the PhD among medical doctors"*

E.L. Fosbøl, P.L. Fosbøl, S. Rerup, L. Østergaard, M.H. Ahmed, J. Butt, J. Davidsen, N. Shanmuganathan, S. Juul, and C. Lewinter (BMC Medical Education, 16 (2016) 189-195)

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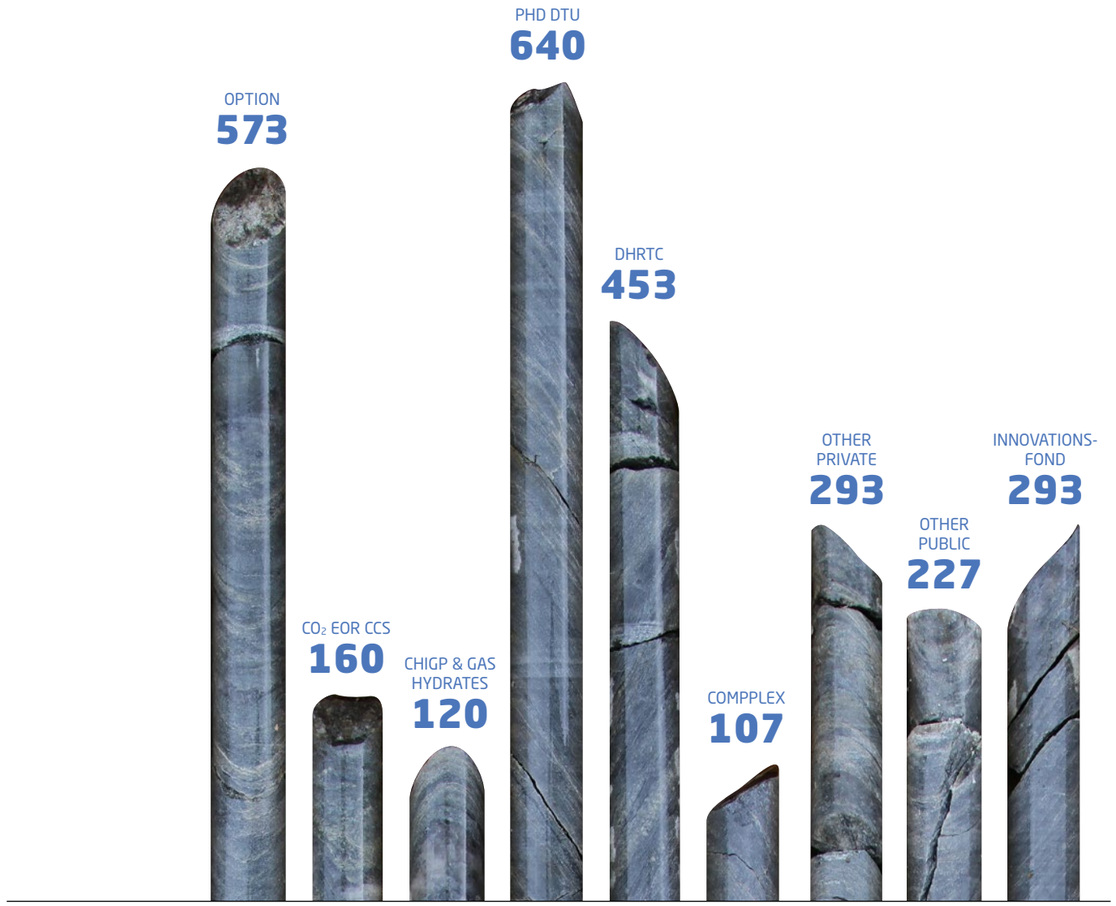

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