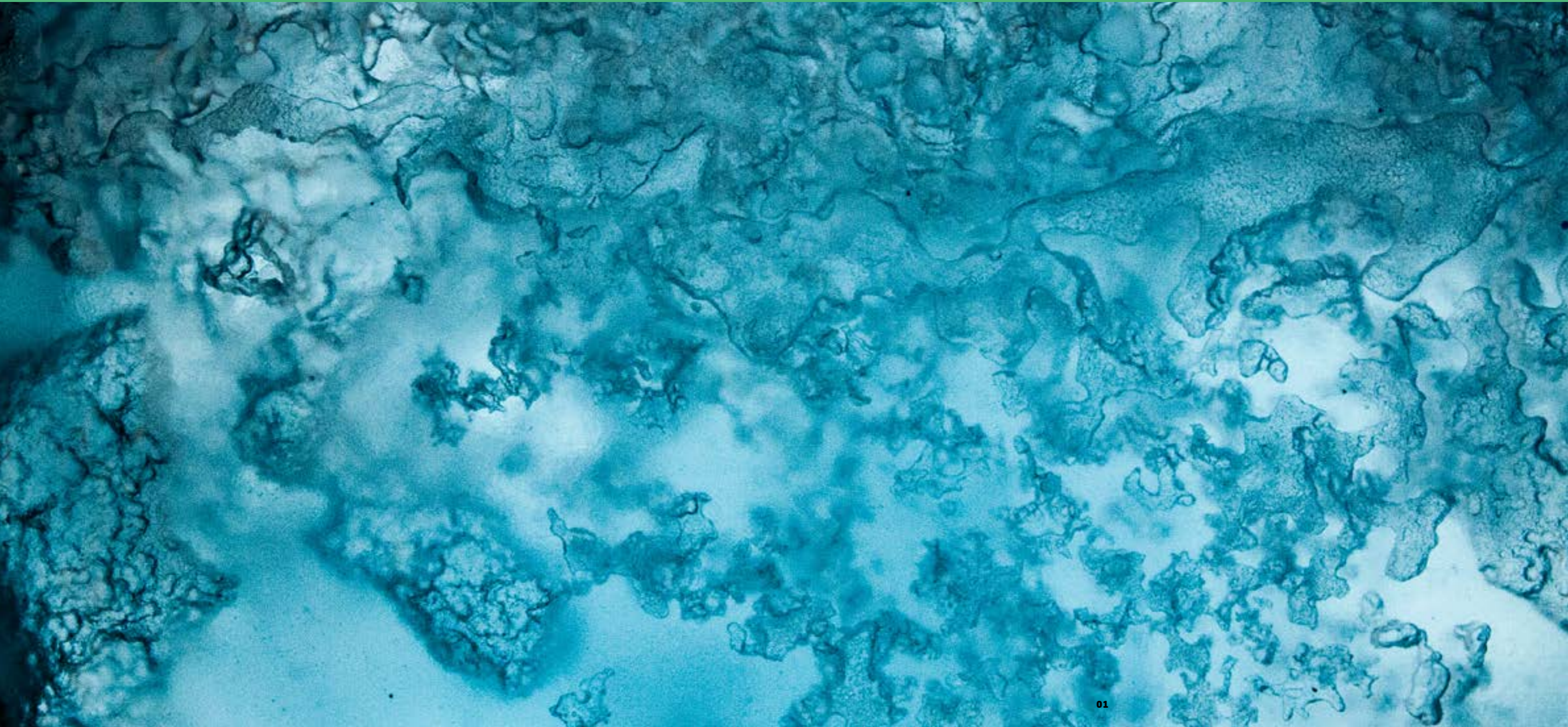




CERE

Annual Report 2018



CERE Annual Report 2018**Publisher**

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We Love People

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Cover photo

Methane hydrates forming in a high pressure stirred vessel. These experiments help us understand the process of forming and melting gas hydrates with a view to producing this vast naturally occurring resource. As an additional benefit these same hydrates can be used to store carbon dioxide, thereby mitigating the effects of climate change.

Diversity and Re-union

While oil & gas research remain important, 2018 saw a further widening of CERE's portfolio and revival of a collaboration with KT Consortium, a cross-center unit of DTU Chemical Engineering.

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This year, the annual main event in CERE set a new record with 117 participants.

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Subsea Gas Dehydration

Assisting Equinor (formerly Statoil), research at CERE contributes to a strong trend in offshore oil and gas exploration: building treatment facilities at the sea bottom rather than on rigs or onshore.

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The World continues to crave Oil

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PhD Theses of the Year

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

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Funding

Diversity and Re-union

Another exciting year has been completed at CERE. 2018 brought many successes and some innovations, but also a few things we would have liked to be different or to change in the coming year.

A major event during 2018 was the Discussion Meeting of CERE, as always well-attended, where researchers from the center presented their achievements and results to the Consortium. This year, CERE's Discussion Meeting was held in partial synergy with KT-Consortium, which is a cross-center unit at DTU Chemical Engineering specializing in computer aided process and product design and process simulation. While today CERE and KT-Consortium have somewhat different targets and structures, both include industrial consortia which started almost 40 years ago from the same single consortium. Thus, it felt natural to attempt this experiment which included a joint poster session, and one common plenary session. The experiment was broadly considered successful and will be repeated during the Discussion Meeting of 2019.

In 2018, one of the center's large interdisciplinary projects, OPTION, reached completion. Over the years, we have enjoyed several of these projects where the diverse disciplines of CERE have been put in action. We hope to be able to start more large interdisciplinary projects in the future. Due to changes in the Danish oil & gas industry and other factors, this has not been easy during the recent years. Still, oil & gas research will continue to play a very important role for CERE. Most such projects with local flavor are now being carried out in close collaboration with DHRTC (Danish Hydrocarbon Research and Technology Center). The CERE-DHRTC collaboration is extensive and we believe it can be further enhanced in the future. We are especially keen to see CERE researchers from various departments participate in broader projects requiring expertise from diverse disciplines, which is one of the strengths of CERE.

Some oil & gas projects are being carried out with Consortium member companies. An example is the cooperation with Equinor (formerly Statoil) described in the current report. CERE's researchers are eager to engage in more industrially-inspired activities and we firmly believe that oil & gas research will continue to be much needed in the years to come.

Carbon capture, bio-refining and ionic liquids

While petroleum activities have always been a major part of CERE's research portfolio, a characteristic of the activities over the recent years is the broad diversity, something we expect to continue in the coming year.

CO₂ capture, utilization and storage has been a major field of research for CERE over many years and continues to be so, not least since CCS has recently re-entered the societal agenda due to the broadly accepted link between CO₂ emissions and climate change.

Another area where CERE will be even more active in the future is that of bioenergy and biorefining. Associate professor Hariklia Gavala is a new faculty from the Department of Chemical and Biochemical Engineering now associated with the center, and we expect that she will further develop this field also bridging to other areas of CERE e.g. the field of bio-thermodynamics. We welcome Hariklia to the center and a presentation of her activities can be found in this report.

We have always been interested in exploring fields which may not be mature but where exciting new applications may emerge; some of these fields of relevance to the strategic areas of CERE, others not.

The field of ionic liquids is one of them, which is of interest to numerous researchers all over the world, maybe not as yet with many industrial applications. We have several projects involving ionic liquids at CERE, and we would be most interested in obtaining the opinion from our Consortium on these and

possibly other areas where they may consider ionic liquids to be of potential use.

Diving into the structure of water

Another field we have embarked over the last years, with funding from Villum Foundation, is the exploration of the structure of water and its link to properties and applications, including possible effects from external (electromagnetic) fields. This is not an area without controversies but we are interested in exploring it, as besides its importance in new applications it may have implications in some of the strategic areas of CERE.

Finally, we welcome two new member companies in CERE Consortium, DSM and Wintershall, officially from 1.1.2019.

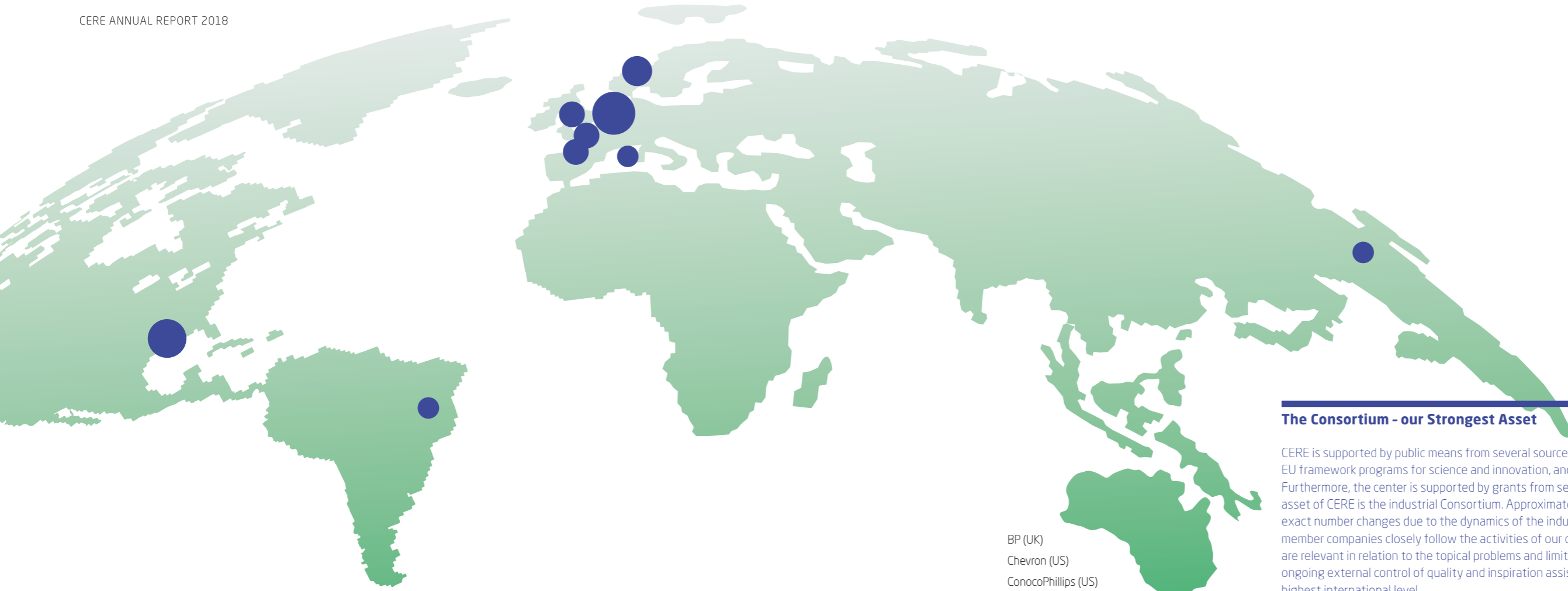
We look forward to the communication and collaboration with all member companies during 2019 and we welcome any comments and suggestions to this annual report and CERE's future research activities in general.

We also hope to see you at the annual CERE Discussion Meeting 2019 in June!

The Discussion Meeting is in itself a major deliverable of CERE where member companies meet CERE faculty, researchers, PhD students and of course each other, can follow all research in a concentrated way and influence, if so desired, the on-going and future research of the center. See you all in June 2019!



Professor
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The CERE Industrial Consortium

- BP (UK)
- Chevron (US)
- ConocoPhillips (US)
- DSM (NL)
- Equinor (NO)
- ExxonMobil (US)
- Haldor Topsøe (DK)
- Hess (DK)
- IFP Energies Nouvelles (FR)
- KBC (UK)
- Linde (DE)
- MOL (HU)
- National Oilwell Varco (US)
- Neptune Energy (UK)
- Nouryon (NL)
- Pentair (DK)
- Petrobras (BR)
- Schlumberger (US)
- Shell (NL)
- Sinopec (CN)
- TOTAL (FR)
- Welltec (DK)
- Wintershall (DE)

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.

We welcome

Wintershall

Operating 26 offshore installations in the North Sea, Wintershall Noordzee B.V. headquartered in Rijswijk, The Netherlands, is one of the larger producers of natural gas in the Netherlands. In 2017, the first oil field operated by Wintershall Noordzee in the Danish sector of the North Sea, the Ravn field, began. Wintershall Noordzee holds three more licenses in the Danish North Sea. Wintershall Noordzee is an advocate for sustainable energy sources, but strongly believes that until there are sufficient sustainable alternatives available, the use of natural gas is an effective method to reduce CO₂ output.

DSM

Royal DSM is a global science-based company in nutrition, health and sustainable living. Originally a Dutch coal mining company, DSM has evolved over more than a century into playing a major role in the shift to renewable energy. The company is highly active in decarbonizing electricity supply both through development of more efficient and sustainable solar modules, and in development of supporting technologies for wind turbines. Further, DSM sees significant commercial opportunities in advanced biofuels and in renewable chemical building blocks, pioneering several advances in biomass conversion. World-wide, the corporation employs approximately 23,000.



From left:
Jean-Charles de Hemptinne,
IFP Energies Nouvelles,
Niels Lindeloff, TOTAL,
Jim Bennett, Schlumberger,
Andreas Grenner, Linde.

The CERE Discussion meeting 2018

As always, the 2018 version of the CERE Discussion meeting was well attended by industry – no less than 23 participants from the Consortium attended. Further, 28 participants from other research institutions and DHRTC were present, contributing to the record overall participation of 117.

The CERE Discussion meeting 2018 was held June 18-20 at the Rungstedgaard Conference Center. A part of the meeting was co-organized with another cross-center activity at DTU Chemical Engineering, the KT Consortium, mainly focused at process and product design and simulation (Process Systems Engineering).

Glimpses of the Discussion Meeting

An impressionistic summary from three days, where industry consortium members and CERE researchers met for mutual inspiration.

The annual Discussion meeting is the time where members of the CERE industry Consortium engage in discussions with the staff of the center.

Smilingly, Dr. Jean-Charles de Hemptinne of IFP Energies nouvelles labels himself as a salesman at this year's CERE Discussion meeting.

"We are inviting both industry and academia to become partners in an upcoming project on electrolyte thermodynamics. This conference offers a nice crowd for selling the idea."

IFP Energies nouvelles is a longstanding member of the CERE industry Consortium and partner in numerous projects. As for Dr. de Hemptinne, he has attended several Discussion meetings but not during the most recent years.

"We try to rotate, so different members of our thermodynamics group get the chance to participate. But participation is definitely a priority. In my view, CERE is one of the only two, or maybe three, consortia in Europe functioning really well within chemical engineering."

A shared devotion to thermodynamics

Uniquely, IFP Energies nouvelles has a leg in both the academic and the industry camp. It is a private group created by the French state and relying on both public and private funding. A majority of the private income originates from sale of subsidiaries, based on license agreements for patented inventions.

Jean-Charles de Hemptinne is in the 15 permanent staff thermodynamics group. The group provides assistance to colleagues engaged in a wide range of applications.

"Our fundamental interest is quite similar to that of CERE. We also share the devotion to applying the thermodynamics. Still, we do cover a wider range of applications – fields like mixed solvents, biomass processes, corrosion issues or batteries to name some," says Jean-Charles de Hemptinne.

"Historically, we have been in CERE because we – like CERE – came from hydrocarbon applications. But today, as indicated by the "Energies nouvelles" in our name, we are active in a number of other energy applications, including bio-energy. Our activities concern both upstream and downstream businesses. Thus, I am happy to see CERE and the KT-Consortium getting closer."

Fruitful mixture of competences

Dr. Niels Lindeloff has attended CERE Discussion meetings previously. However,

he represents TOTAL for the first time here after TOTAL's recent acquisition of Maersk Oil.

"TOTAL has been a member of CERE for many years. We find the combination of CERE's strong background in thermodynamics and the inclusion of competencies from other disciplines fruitful. For instance, it is not possible to fully develop Enhanced Oil Recovery without an understanding of the geoscience involved. Also we would like to understand the history of reservoir formation on geological time: How the different physical and chemical processes resulted in the current variation of the properties of reservoir fluids."

Niels Lindeloff encourages CERE to maintain the current balance between chemical engineering and geoscience disciplines:

"The strong history and competence within applied thermodynamics is the main selling point of CERE. One always needs to be careful not to dilute ones' core competence. We find the interdisciplinary approach extremely useful, and still see the role of the other disciplines to be leveraging application of thermodynamics to solve relevant challenges."

Clients face increasing complexity

Dr. Jim Bennett of Schlumberger attends the CERE Discussion meeting after a three-year break.

"Before that interval I was here three years running. But I guess it is good to miss a few years and come back with a fresh view. The most apparent change is all the students being new. Still, I find a lot of continuity."

Schlumberger is the worlds' largest engineering consultancy company within energy resources applications. With a

background in mathematics, Jim Bennett specializes in modeling of the behavior of fluids in reservoirs and during oil and gas production.

"For complex and expensive wells modeling becomes more important. Also, being able to handle water in the models is a focus. Especially at the wells, we see large amounts of water in the gas phase. This introduces a different level of complexity to the modelling."

Being consultants, Schlumberger always tries to stay ahead of the clients' needs.

"Some clients are taking increasing interest in asphaltenes. This is a field where I feel the current simulators are lacking behind. The task is challenging since it involves thermodynamic modelling for multiple phases."

Asked whether he has found inspiration for his daily work at the Discussion meeting, Dr. Bennett gives a dual answer:

"I definitely return with new ideas, but my problem is to find the time to elaborate on them. In recent years, we have had to do less research and more development. For instance, I would love be able to do some joint projects with PhD students, but it doesn't seem possible right now."

Returning in new capacities

During his closing remarks at the Discussion meeting, CERE Chairman Georgios Kontogeorgis notes the continuity represented:

"It is a great pleasure to see that no less than 25 % of the industry participants here are former master students, PhD students or postdocs of CERE. We are always happy to see our alumnae again.

Having them here as representing industry shows the vitality of CERE and the industry Consortium."

In the contingency of people returning in a new capacity is Dr. Andreas Grenner of Linde Engineering Division:

"A few years back I was a postdoc with CERE, but this is my first Discussion meeting at the industry side of the table."

Linde Engineering focusses on segments such as plants for the production of hydrogen and synthesis gas, oxygen and olefins as well as plants for natural gas treatment.

"In all these applications, thermodynamic modelling is highly relevant. I come here to be inspired both in terms of model development, new software, and ideas for potential collaborations. CERE is recognized as one of the leading chemical engineering groups in Europe. That's also what motivated me to take a postdoc position here."

Besides his new role as industry participant, Andreas Grenner points to another novelty this year:

"I find the new concept of combining the CERE content with contributions from the KT-Consortium interesting. It seems apparent that both consortia have similar interests. Yet, they also have some differences in their angles which may introduce new ideas both ways and create synergy. It is always healthy to get different perspectives. Having a joint event is definitely a good thing."

Contributing to the Subsea Revolution

With offshore oil and gas exploration trending ever further offshore and ever deeper under the sea, there is an increasing drive to build treatment facilities at the sea bottom rather than on rigs or onshore.

The animated videos found at the website of Equinor (formerly Statoil) seem to come from a science fiction movie. As the virtual camera slowly pans across still more yellow-painted steel installations, the image of a space colony at a remote planet comes to mind. Yet, we are here at Earth, but at the bottom of an ocean. Today, it is quite possible to develop an offshore oil field without any rigs visible at the sea surface. Actually, half of Equinor's production comes from 500 subsea wells. Not surprisingly, this requires more than development of novel subsea facilities. To design these facilities, extensive efforts within thermodynamic modelling and experimental measurement campaigns are highly needed.

"Repairing or replacing equipment at the bottom of the ocean will be extremely costly. So, you need to do your homework carefully and get it right the first time," says PhD student Francois Kruger, CERE. "The most important role of CERE in this respect is to replicate what Equinor is doing. Our equipment here at DTU is similar, yet slightly different. So, we can provide valuable verifications of their results."

The collaboration with Equinor dates back some 20 years. Most of the work has been under the umbrella of the CHIGP (Chemicals for Gas Processing) Joint Industry Project. In total, five PhD projects have been sponsored by the Norwegian energy corporation, with Francois Kruger's project as the most recent.

Longer pipelines become possible

The project focusses on subsea gas dehydration (water removal). In 2015, Equinor inaugurated its Asgaard Subsea Gas Compression facility – the world's first facility of its kind.

Compression is a key part of the water removal process. During offshore oil and gas production, water contamination is unavoidable. Traditionally, the water

is removed at a later stage, but doing it already at the sea floor has several advantages, Francois Kruger explains: "First of all, transporting a mixture of water and gas puts constraints on the length of your pipeline due to the risk of problems such as slugging and gas hydrate formation. If you can instead transport pure gas, these problems are minimized. So, you will be able to increase the length of your pipeline significantly meaning you can reach resources further away from your central treatment facility."

Another advantage is improved energy efficiency. "In the deep reservoirs, the gas is under high pressure. This is actually handy in respect to removal of water. Under high pressure, the water will tend to separate without any further measures. But if you – as traditionally seen – transport unprocessed gas over several kilometers, the pressure will drop. You will need to either invest energy in getting the pressure up again, or use intensified processing, also requiring energy consumption."

Large savings on chemicals

Further, dehydrating the gas at the sea floor reduces the need for addition of chemicals. In traditional offshore recovery, chemicals are added for gas hydrate inhibition to prevent pipe blockages leading to serious downtime. For many years, methanol was predominantly used. Today, glycols such as MEG are preferred.

"The environmental profile of MEG is superior to methanol, yet it is obviously desirable to limit its use. This is not just for environmental reasons, of course, but also economic," says Francois Kruger.

By removing the water already at the sea floor, the amount of MEG needed for gas processing can be limited to as little as 1/6 of the amount used in traditional applications.

The savings not only come from the price of the chemical itself:

"Everything we put into the gas will need to be taken out again later, before the final product reaches the customers. So, when we put less into the gas in the first place, we will save on the later stages of gas treatment."

The experimental campaigns at CERE involve advanced equipment such as a three-phase equilibrium cell and a new gas chromatograph, Agilent 7890B, for

quantification of the various fractions and their phase distributions. The experiments are able to measure data for complex mixtures of hydrocarbons, water and MEG up to 150 bar and 50 °C.

Further, Francois Kruger has developed a modification for modelling of MEG within the CPA (Cubic Plus Association) thermodynamic model.

The tools developed in the project are made available to Equinor and the other CERE industry consortium partners with implementations available in MatLab and AspenPlus.

Know your level of uncertainty

The end-goal is creating tools that may assist operators in deciding the specifications for design of actual subsea facilities.

A significant novelty in these tools is the use of an uncertainty analysis technique, known as bootstrapping.

"Traditionally, a model would predict a certain value for a given output parameter. But we have found that it is actually helpful for a company to not just have an estimated value, but rather an interval. Due to the high economic risk involved in subsea installation, you want to make sure that not just the most likely value but the full interval of possible values lies within the acceptable limits," explains Francois Kruger.

This may sound like adding to costs, but that is not necessarily the case:

"Industry practice does obviously not accept a value just within the safety limit as acceptable, but will include additional, generic safety factors. However, if we are able to demonstrate that all possible values are well within the safety limit, it might be possible to use smaller safety factors and still stay within the safe operating region."

This may lead to additional advantages:

"If you apply unnecessarily high safety factors, you are not just adding to costs. Operating at strict conditions can actually be quite harmful to your processes leading to unnecessary consumption of energy or chemicals."

Optimization of Production from Oil Fields

A highly interdisciplinary four-year Joint Industry Project has taken optimization of production over entire oil and gas fields to a new level.

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

“We set a highly ambitious goal four years ago, and we have shown it could be done. Through advanced mathematics it is actually possible to make a difference in oil and gas recovery,” says Allan P. Engsig-Karup, Associate Professor at DTU Compute and member of the CERE Faculty.

From the outset it was clear, that the project would be highly challenging.

“We knew we not only needed to tackle the mathematical and computational challenges introduced by the various well locations

and production rates, but also the large uncertainties related to the underground. While we may have some ideas about how the geology looks and which processes take place, we cannot know for sure. This complexity can only be addressed through a high degree of interdisciplinary cooperation. The combined knowhow from industry and academia proved a strong base for synergy within the project,” says Allan P. Engsig-Karup.

Since the perspective is increased oil and gas production from a field, and thus higher potential economic gain, it is natural to ask why individual energy corporations have not already done something similar?

“The computational challenges are really large, even with the resources available to international energy corporations. One of the problems to face is the fact, that while you may be able to purchase relevant software, this will not get you all the way since such tools are not prepared for the kind of investigations done in OPTION. You need access to the software code itself, something which is not possible for commercial software packages. Open source software provides access to the code, and this may help improve things. So ideally, you want to bring the best from both worlds together. With our specialists’ insight we chose a path where we developed the relevant computational tools ourselves and enabled taking advantage of any tool that could help achieve our targets,” Allan P. Engsig-Karup explains.

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

“Our priority was to get the physical modelling right in terms of first principles and then we developed smarter algorithms which would allow us to do calculations faster without sacrificing accuracy. To that end we followed a dual approach. On the one hand we would do a full, expensive simulation using established tools that could serve as a means for validations, and on the other hand experiment with developing the new algorithms. We would then compare with the full simulation and evaluate if the faster and cheaper solutions were satisfactory. This strategy of using the established tools ensured that we could find ways to improve the established practice,” says Allan P. Engsig-Karup.

“Actually, we already see new opportunities for finding additional shortcuts which would bring down computational costs further. This would increase the chances for the developed solutions to be implemented in practice. We aim for addressing this in future spinoff projects.”

Producing more Oil, and less Water

Lloyd’s Register recommends for its energy industry clients to implement results from the OPTION project: more oil and gas can be produced.

By coupling Computational Fluid Dynamics (CFD) with reservoir modelling, more accurate representation of hydrocarbon producing wells and their surroundings can be achieved. This is the most interesting result from the OPTION project, according to one of the industry participants.

“More accurate modelling allows for designing the wells better. This again translates into producing more oil and gas, and less water, over the life time of a field,” says Kenny Krogh Nielsen, Team Leader and Senior Principal Consultant in fluid dynamics, Lloyd’s Register.

Lloyd’s Register is a global engineering firm specializing in advanced simulation technology for the design and analysis of complex structures and systems. The branch in Aberdeen, Scotland, has world-class expertise in CFD modelling for the oil and gas industry, including a patent and the trademark Well-scope.

“We were encouraging CERE to start the OPTION project, because we saw a perspective in combining our CFD knowhow with the competences of CERE, not least within reservoir modelling. This has actually been accomplished,” notes Kenny Krogh Nielsen.

Clients have already benefitted

Typically, a hydrocarbon reservoir will have a layered distribution with oil, gas, and water separated due to the differences in density. The task is to produce the hydrocarbons with minimal amounts of water entering the production stream.

“If you have designed your well poorly, you will soon begin to produce water, and as time goes by the proportion of water in relation

to hydrocarbons increases. Even though you are still producing hydrocarbons of high value, you may eventually be forced to abandon the well, simply because you cannot boost your water management system sufficiently to handle the large amounts of water produced,” says Kenny Krogh Nielsen.

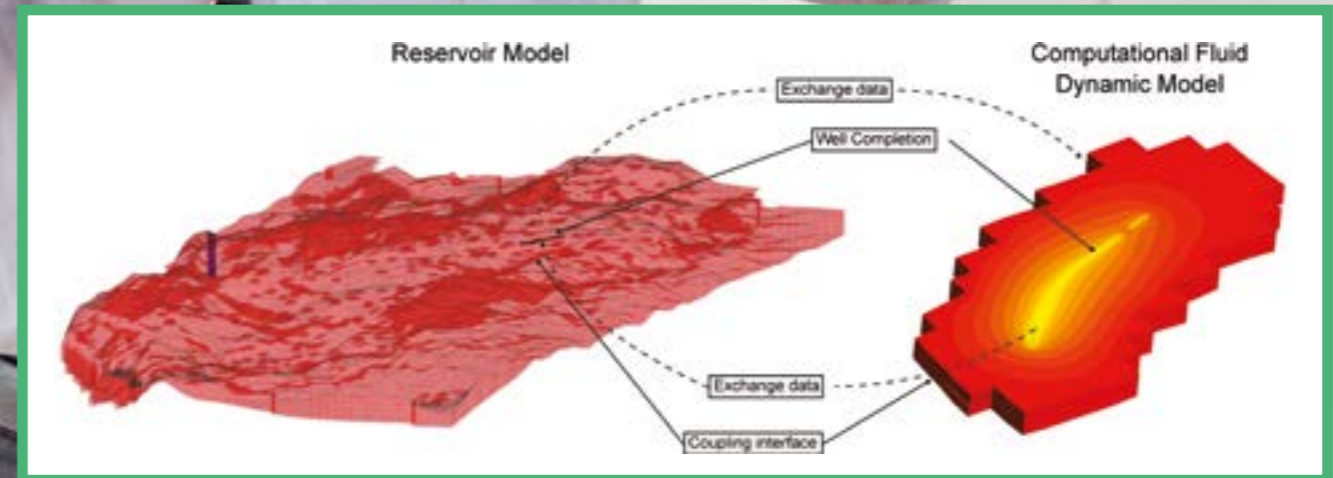
This illustrates how important the initial well design is in relation to the expected production and net value of hydrocarbons over the life time of a reservoir:

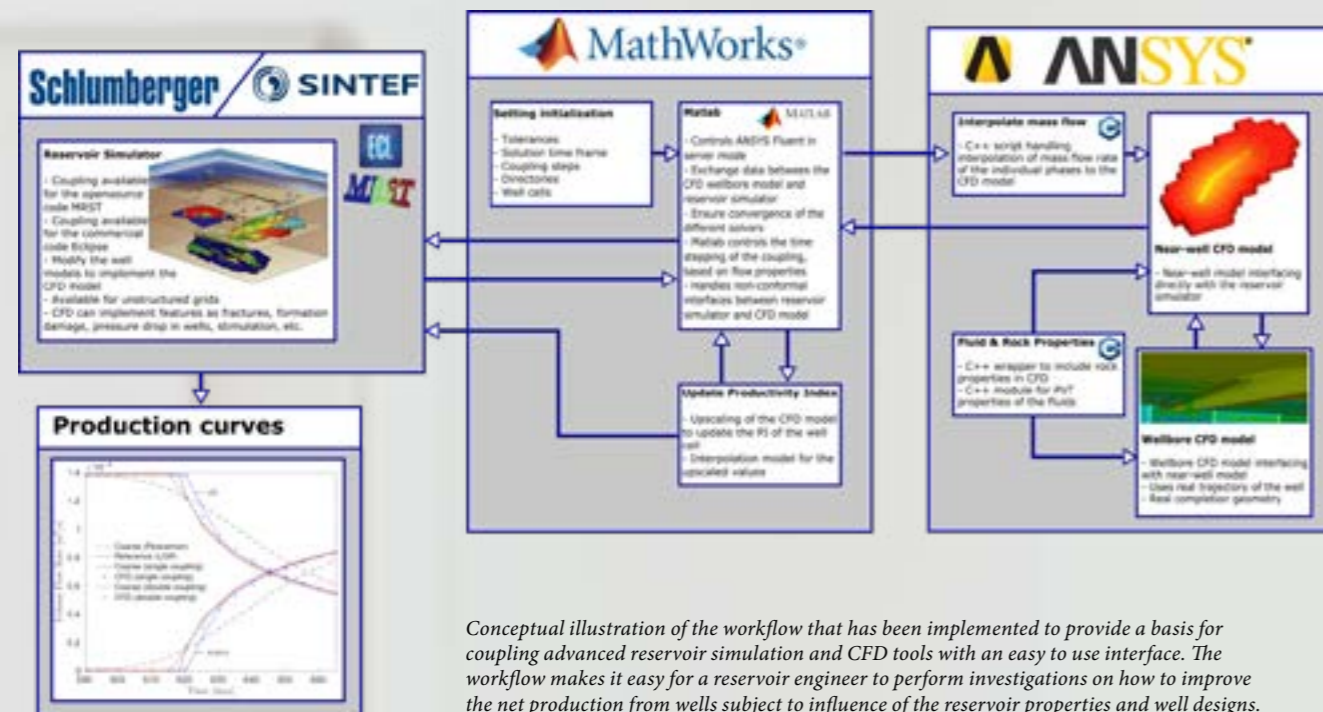
“If you look at the Danish part of the North Sea, production is typically from horizontal wells running maybe 2 or 3 km below the surface. While you may have some ideas about the conditions down there from seismic data and similar sources, a high degree of uncertainty is involved. From my perspective, it is quite obvious that you can benefit from combining well flow modelling with reservoir modelling. Some uncertainty will still exist, but you will be able to come much closer to the real situation. Already, we are able to state that in this way some of our clients have been able to save costs and earn more.”

A cautious type of industry

To an outsider, it would seem like the extra production and net value would motivate the entire industry to adapt the OPTION results the sooner, the better.

“I expect to see this approach spreading, but it will take some time. This is a conservative





Conceptual illustration of the workflow that has been implemented to provide a basis for coupling advanced reservoir simulation and CFD tools with an easy to use interface. The workflow makes it easy for a reservoir engineer to perform investigations on how to improve the net production from wells subject to influence of the reservoir properties and well designs.

industry!” Kenny Krogh Nielsen says, smilingly. He admits that people in the industry have good reason to be cautious:

“In other industries, you have much better conditions for being innovative. For instance, in the car industry you could just manufacture two different vehicles that were identical except for the one feature you are interested in, and then take them for comparative tests. As the cost of a new well lies in the 50-100 million USD range, you don’t just make an extra well for reasons of comparison. And even if you did, the geology wouldn’t be exactly the same. In other words, we can never provide absolute in-situ proof of our suggested approach being better. However, the rigorous modelling investigations provide strong indications.”

A further hindrance is the general secrecy in the industry.

“Energy corporations are reluctant to share data concerning their reservoirs. This is quite natural, because if you tell your competitors too much about your reservoir, they may use that information to win the next public tender for that area. Further, publicly traded companies are not able to share potentially important financial information that may interfere with the valuation of the company on the stock market. But while the wish for discretion is understandable, it does

conflict with the desire to compare various well design concepts and clarify which are better.”

Going deeper into the science

To understand how the combination of CFD and reservoir modelling can improve production, it is worth moving a bit deeper into the scientific substance in OPTION. Near-well flow analysis is an important tool for improving well design and optimizing oil and gas production. However, the scale disparity factor in space and time is a challenge. The numerical scale gap between the reservoir and the wellbore justifies the representation of a well as a point or line source term in traditional reservoir models. However, standard numerical techniques for reservoir simulation are incapable of resolving the near-singular character of the pressure field in the vicinity of the well.

Under the assumption that all length scales have impact on flow patterns, the researchers in the OPTION project have improved the quality of the numerical simulation by considering the geometry and fluid flow near the wellbore in a fully connected system, thus accounting for the fine scale phenomena by means of a well bore model (hybrid Navier-Stokes/Darcy) coupled with a full-scale reservoir model. Several numerical experiments have been performed, demonstrating the versatility

and improved well performance insight offered by the coupled method, including horizontal well inflow profile, influence of formation damage, and optimal well configuration.

An accomplished mission

Apart from plain conservatism, an argument against the OPTION approach might be the costs of computing.

“Now it is true that if you are determined to do full scale simulations, the computation time does become an issue. Possibly, future projects may find shortcuts that allow for shorter computation time. Also, we have found that you can typically do partial simulations, that will give you largely the information needed for your well design,” says Kenny Krogh Nielsen.

The Aberdeen branch of Lloyd’s Register has already implemented such solutions in collaboration with international clients. Further, a full-scale demonstration project within the OPTION project will soon be completed in collaboration with Ineos in the Danish part of the North Sea. Ineos has acquired the hydrocarbon activities of the former DONG Energy, partner in OPTION.

“Right from the beginning, as we co-initiated the OPTION project, we were keen to see a

scope that would lead to development of new technology and software,” says Kenny Krogh Nielsen. “Implementation was the intention from day 1, and at the completion of the project we can note this to have been largely accomplished.”

New Perspectives for Well Completion

As a leading supplier of well equipment for oil and gas recovery, Welltec is keen to implement results from the OPTION project.

Reservoir simulation models used for optimization of oil and gas recovery are in general solely based on reservoir parameters, whereas the flow regimes near the well bore and inside is simplified in the simulations. The complex flow regimes in vertical, deviated and particular horizontal well is however well understood by the use of Computational Fluid Dynamics (CFD). Furthermore, the ongoing production can be optimized cost effectively through an iterative simulation based on realized production data. This has been the main tasks of the OPTION project.

“The project has yielded results which none of the participants could have achieved alone,” says Mette Fürstnow, Business Development Manager at Welltec, one of the industry partners. Welltec is a leading supplier of well equipment for oil and gas recovery.

In relation to the OPTION project, especially the company’s Well Completion Solutions have been in focus. These solutions are built to provide operators the flexibility to design and run the optimal completion for their reservoirs. Welltec’s annular barriers are affixed to a large, full bore completion liner and used to divide the well into compartments dictated by geology to achieve optimized production of hydrocarbons through Life of Well reservoir conditions.

First participation in joint research

OPTION marks the first participation of Welltec in a Joint Industry Project with other private companies and public research groups.

“In the sense that the results from the project would probably not have been produced – not by us, nor by any of our competitors – without the Joint Industry Project, it has been successful. Still, as a private enterprise you always hope to come even further,” comments Christian Krüger, VP, Marketing & Sales, Welltec.

“We were maybe overly ambitious, but we actually had hopes of seeing ready-to-use

commercial products by now. We are not the ones to capitalize directly on the OPTION findings. This is more the role of another industry participant, Lloyds Register, as they provide consulting to their clients. However, we hope to have access to the OPTION based and developed relevant software in our sales and design phase to ultimately deliver better advice and better solutions to our customers.”

Better understanding of flow through wells

The OPTION work packages have fulfilled most of their various goals, according to Mette Fürstnow:

“However, the overall integration of results across the work packages has not been completed to date. I know the researchers wanted to get to that point, and they are keen to continue these efforts, and hopefully they will succeed. Until the partial results are integrated into an overall solution, we cannot use the results directly towards our clients. Even so, the project has provided us with an improved understanding of

flow through wells, and how it can be modelled. This, along with a strengthened collaboration with Lloyds Register will benefit our efforts within well completion sale long-term.”

“One lesson we have learned is to be more focused on project management. Over the project period of four years, including a severe downturn in the oil industry, several key people in OPTION left and others came on. Changes which should be expected in a dynamic environment and which Welltec and the other participants would be ready to handle better another time.”

Christian Krüger concludes: “Should the possibility of taking part in a similar project in a similar setup arise again, we would be very positive.”

Allan Peter Engsig-Karup
Associate Professor

The OPTION Project

The scope of the OPTION project (Optimizing Oil Production by Novel Technology Integration) is to increase the understanding of the interface between reservoir and well performance to improve well and completion design to enhance productivity and oil recovery. OPTION is led by CERE and integrates a range of disciplines across DTU. It is supported by a close to 2.0 million EUR grant from the Danish National Advanced Technology Foundation. Industry partners are Welltec, Lloyd’s Register, and Ineos. The total budget is 4.0 million EUR. Professor Erling H. Stenby, CERE, has coordinated the OPTION project.

Thermodynamic Control Tools as Open Source

Process system tools such as Nonlinear Model Predictive Control (NMPC) are widely used in the process industries for development of operational strategies and control for process systems. These tools rely on thermodynamic models. However, traditional thermodynamic models are generally intensive in terms of computing capacity. Further, they are typically not available as open-source. A research team at CERE has changed this picture with the development of a novel open-source rigorous thermodynamic library, which is designed for dynamic simulation and optimization of vapor-liquid processes.

PhD Student Tobias K. S. Ritschel, Postdoc Jozsef Gaspar, Postdoc Andrea Capolei, and CERE faculty, Associate Professor John Bagterp Jørgensen, have contributed to the scientific article entitled “A Thermodynamic Library for Simulation and Optimization of Dynamic Processes.” Published in IFAC-PapersOnLine, the article makes the new library available to users.

The new library is implemented in Matlab and C and uses cubic equations of state to compute vapor and liquid phase thermodynamic properties. As a novelty, it also provides analytical first and second order derivatives. These derivatives are needed for efficient dynamic simulation and optimization. The analytical derivatives improve the computational performance by a factor between 12 and 35 as compared to finite difference approximations.

New faculty member

Bio-energy Resources Engineering Associate Professor Hariklia Gavala strengthens the profile of CERE within the biological aspects of energy resources engineering.

With biological feedstock contributing increasingly to energy supply, biological processes become still more important to energy resources engineering. Associate Professor Hariklia Gavala has more than 20 years of experience as a researcher and research manager within bioprocess engineering.

“During the last few years, I have worked in collaboration with CERE researchers. While CERE generally has its strongholds within applied thermodynamics, I have contributed with biological knowledge. The synergy goes both ways. I often find knowledge of thermodynamics to be very helpful in bioengineering. For instance, if you want to predict the yields of products from a biological process, you may need to include thermodynamics in your simulations. We have also proved that thermodynamics can be used as a tool to direct microbial enrichments towards desirable products. As a faculty member in CERE, I look forward to developing this collaboration even further.”

Hariklia Gavala has expertise on anaerobic digestion, fermentation processes with pure and mixed microbial consortia, pre-treatment methods for biomass exploitation, kinetics and modelling of biological processes and membrane

applications in biorefineries. Her research has a strong focus on biological processing of biomass resources for sustainable production of biofuels and chemicals.

Mixed microbial consortia cut costs

In relation to CERE, Hariklia Gavala has been strongly involved in SYNFERON (Optimised SYNgas FERmentation for biofuels production) since the initiation of this project in 2015. One route in production of bio-energy is generation of “syngas” - which is a mixture of H₂, CO₂, and CO - through gasification of biomasses. The syngas can be used in combined heat and power production. In the SYNFERON project, the syngas is fermented to liquid (alcohols) and gaseous (methane) biofuels which can easily be stored or transported.

“As fermentation is a microbial process, the bio-conversion component has been at the core of SYNFERON all the way through,” Hariklia Gavala states.

Some biotech applications rely on pure microbial cultures, where a single microbial species is used - often in a genetically engineered version - to perform a very specific job. For instance, this is a common choice in the pharmaceutical industry. In contrast, the bioprocessing tasks in SYNFERON rely on mixed microbial consortia and thermodynamically driven enrichment processes and reactor operations.

“Pure cultures require costly procedures, for instance sterilizing equipment and feedstock to avoid contamination from other species. This can be justified if you manufacture a high value product like medicine, but for low value products like

ethanol and methane you need something cheaper,” she explains.

New reactor for methane production

However, using mixed microbial consortia is not just hoping for the best. On the contrary, the team has recently achieved significantly higher yields and productivities of methane and other biofuels by using enriched microbial cultures.

“The results have been encouraging, and we are beginning to disseminate our findings in scientific publications. At the same time, we are taking things a bit further. We have achieved good results in the lab, but we want to apply the methods to pilot reactors and show that they also work in continuous production.”

The project involves a collaboration with the Pilot Plant unit and the PROSYS center at DTU Chemical Engineering. In an effort headed by Associate Professor Ioannis Skiadas, a trickle bed reactor which results in high methane yield and productivity has been developed.

A further effort relates to production of alcohols, i.e. ethanol, from syngas.

“We have shown the possibility to produce ethanol from mixed microbial consortia. This can be done either in a traditional suspended system or in a reactor of the trickle bed type. Further experiments will clarify, which of these solutions is the best,” says Hariklia Gavala.

Hariklia N. Gavala
Associate Professor



“We have shown the possibility to produce ethanol from mixed microbial consortia.”

Associate Professor Hariklia Gavala,
DTU Chemical Engineering

The objective of the SYNFERON project

The objective of the SYNFERON project (Optimised SYNgas FERmentation for biofuels production) is development of a gasification/bio-conversion technology platform. This will include both a novel reactor type, development of designated mixed microbial consortia 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 SYNFERON technology platform would 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 offering several thousand new jobs. Also, the implied increase in the use of residues - including agricultural residues and waste biomasses - can provide an extra income to farmers and/or solve waste treatment problems.

Partners in the SYNFERON project are DTU Chemical Engineering, Danish Gas Technology Centre, Aquaporin A/S, Biosystemer ApS, Highterm Research GmbH (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 SYNFERON project is due to be completed in its present form by summer 2019.

The Comeback of Carbon Capture

Following some years of stagnating public funding, the interest in limiting carbon emissions from industrial and energy production facilities is on the rise.

Moving from fossil to renewable energy forms will probably not be enough to preserve the planets' climate. Some level of carbon capture will be needed as a supplementary measure. This observation from the UN climate panel IPCC and other authoritative bodies has brought fresh vitality to the field of Carbon Capture and Storage (CCS). For instance, the Danish government has announced a 100 million DKK scheme for climate protection.

"This is the first time we see a genuine Danish investment in CCS activity, not just money for basic research," notes Associate Professor Philip L. Fosbøl, coordinating carbon capture activities in CERE.

The first surge of CCS interest took place some 20 years ago. However, as no efficient international scheme to combat carbon emissions was established, the interest of several governments – including the Danish – cooled down, and funds were instead directed towards green energy forms. Still, some public programs remained, mainly in EU and Norway. Active participation in these collaborations has allowed CERE to maintain its level of research in the field. And for Philip L. Fosbøl personally, this has meant frequent appearances in Danish TV as a national expert on carbon capture.

"To my mind, we will not be able to do without carbon capture. According to IPCC, the world will need not only to get to zero carbon net emissions by 2050. If we are to preserve the present climate, we actually need to achieve negative emissions. Saying negative emissions is another way of saying carbon storage. And storage of course includes capturing."

Capture is really not that costly

The dominant method for carbon capture is by use of amine-based solvents. Extensive research efforts

and pilot plant campaigns have taken the necessary techniques to a mature state and also reduced costs somewhat. Still, the label "costly" seems to stick. This frustrates Philip L. Fosbøl:

"Obviously it costs more to apply CCS than to just go on emitting carbon dioxide. But if you compare CCS to other green technologies, it is actually not expensive. For instance, producing electricity from wind turbines is 2-3 øre/kWh, and used to be 37 øre/kWh. If we use CCS, the cost is 6-8 øre/kWh. This cost is out of a power consumer price of 225/kWh."

This calculation should not be used as an argument for continuing production of fossil-based power in business-as-usual style with just CCS added:

"Certainly not! However, also in a sustainable scenario will we need to produce goods which are bound to emit CO₂. We cannot just stop using steel, cement, medicine, paper and similar types of welfare goods which rely on processes which emit a noticeable amount of CO₂. Therefore, we should invest in CCS just like we have invested significant resources in development of photo voltaic cells, wind turbines, and other green technologies. But I am aware, that we are walking a thin line here. You will always face critique. Some will argue, that carbon capture is a way of keeping the fossil business afloat. It is important that the pace of the transition to renewable energy is kept. We need to pursue a dual strategy to preserve the climate."

A by-product from biogas upgrading

The research group does not only take an interest in capturing CO₂ for storage. The scope of the project "BioCO₂", coordinated by Philip L. Fosbøl, is to capture CO₂ during production of biogas and turn it into a product of commercial value.

"For some years now, production of biogas from manure and other agricultural waste products has caught on. Biogas can be upgraded into methane. This upgrading both increases the energy value of the gas and allows for storage of excess gas in the high-standard Danish storage system for methane," explains Philip L. Fosbøl.

During upgrading of biogas to methane, CO₂ is removed as a by-product. Roughly 35 percent of the biogas is CO₂.

"Unfortunately, it is not possible to use the CO₂ from biogas upgrading directly for the various industrial purposes where CO₂ is in demand. If things were that simple, utilization of this CO₂ would already be in place. Each of the purposes in question have their own specifications, but generally the requirements for purity are very high. It is a key challenge in the project to meet these specifications in an economically feasible way," says Philip L. Fosbøl.

BioCO₂ is a 4-year effort sponsored by the EUDP program under the Danish Energy Agency. Besides CERE, the Danish Gas Technology Center (DGC) and Pentair are partners to the project. The Danish branch of Pentair, Union Engineering, located in Fredericia, specializes in plants for amine-based capture of CO₂.

Portable plant under construction

Together, the partners are constructing a portable plant to demonstrate the BioCO₂ technology. After completion it will be installed for periods of operation at two different locations. One location is Mølleåværket, a sewage management plant operated by Lyngby-Taarbæk Forsyning, and the other is a biogas facility at Fyn operated by Nature Energy.

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

Besides the new production of high-quality CO₂, Philip L. Fosbøl stresses that CO₂ will contribute to fulfilment of the ambitious Danish policy on sustainable energy:

"It seems realistic that methane from upgrading of biogas can substitute 5-7 percent of the current energy consumption in Denmark. If further biomass becomes available, this number could go even higher in the future. Hopefully, BioCO₂ will contribute to this development by making biogas upgrading more economically attractive both to farmers and to biogas plant operators."

Huge potential for utilization

Another area with a large potential for utilization of CO₂ is in synthetic fuels:

"We have seen significant improvements in electric and hybrid vehicles, but some problems in battery capacity remain. Even the best battery cannot compete with fuels when it comes to energy density. This is especially true for airplanes, where the possibilities for recharging batteries during the flight are not really available. This could be an argument for maintaining fluid

fuels for air planes, also in a future sustainable scenario. However, we shouldn't rely on today's fuels which are highly damaging to the climate, but rather develop new synthetic fuels with a much better climate profile. Here, captured CO₂ could be a promising raw material."

A related technology could be utilization of excess wind power for production of either synthetic fuels or hydrogen.

"This would be a way to store excess renewable energy. Admittedly, the energy efficiency in converting power into fuel or hydrogen is quite low. But then again, having an efficiency of, say, 30 % is still much better than just wasting power, meaning zero % efficiency, as is sometimes seen when the wind is strong."

Global CO₂ emissions from industries total 35-40 Giga tons per year, and the current utilization is only 0.2 Giga tons.

"So, there is a huge potential for more utilization. But despite the various ideas for utilization, we will still need to look at storage. In Denmark we do have suitable sites, not least former gas reservoirs."

Underground CO₂ has high density

In several countries, plans for CO₂ storage have been upheld by protests from concerned citizens. For a chemical engineer such protests do seem a bit strange – as CO₂ is emitted in large quantities every day, not only by industry but also by all living creatures, including humans. On top of that, Philip L. Fosbøl notes an argument, which has not really entered the debate yet:

"People seem to think of the stored CO₂ as if it was air, which would rise upwards through any type of crack in the rock. But actually, the density of the underground CO₂ is high. It is heavier than water and will not have a tendency to find its way upwards, but possibly downwards. As the years pass, the surrounding rock will take up the CO₂, which means the CO₂ assumes mineral form, further adding to its stability."

Should these arguments fail to impress, there is still a way forward:

"We have the emptied-out reservoirs in the North Sea. Using them for carbon storage would add to costs due to transportation and maintenance of offshore installations. But at least, no neighbors will object. We basically put the CO₂ back where it came from."

Philip L. Fosbøl
Associate Professor

Carbon Capture at CERE

With the rising interest, CERE expects to expand its CCS group to 5-6 researchers. Further, some 5-6 students are doing projects on carbon capture. Industrial partners include GASSNOVA (Norway), GEUS, Pentair, and Nature Energy.

Among recent achievements are promising results from using vapor reducing agents (VRA's) as solvents rather than amines. The VRA's have been shown to perform as good as the current state-of-the-art amine MEA (mono-ethanol-amine) for capture of CO₂.

"This is highly encouraging. The point is, that the actual capture is only half of the equation: you also need to release your CO₂ again a bit later both in order to utilize or store the CO₂, and to regenerate your solvent. We have every reason to believe that the VRA's investigated will be better at releasing the CO₂, and thus the energy efficiency over the entire process will be better. This is what we will strive to prove in upcoming projects," says Philip L. Fosbøl.

Another prominent project is financed by Norwegian energy corporation GASSNOVA and involves measurements at the Test Center Mongstad (TCM) – the world's largest carbon capture pilot plant with a capacity of 50,000 cubic meters per hour. In comparison, the capacity of the largest pilot plant facility in Denmark – the former facility in Esbjerg – was 5,000 cubic meters per hour.

"If you build something larger than the TCM, you cannot call it a pilot plant. It would be a full-scale facility," as Philip L. Fosbøl puts it.

The aim of the project is to create an extensive understanding of process optimization using a base case MEA solvent for carbon capture. The idea is, that the performance of alternative solvents can be compared with this reference data set.

The EOR Community met in Denmark

For a week in September 2018, Denmark was the center of international efforts to raise oil and gas production rates.

15 countries take part in the Enhanced Oil Recovery (EOR) efforts under the International Energy Agency (IEA). They meet annually to exchange experiences. In 2018, Denmark hosted the conference at a time where EOR is more relevant than ever. For several decades now, Denmark has been an oil exporting country. However, production from the North Sea fields is declining and for the first time since the beginning of Danish production, oil and gas imports are about to exceed exports. Thus, the background was one of concern as representatives of international energy corporations, authorities and researchers gathered at the Schæffergården conference center in Lyngby.

“If we can produce just a few extra percent oil from the North Sea, the value will be billions of DKK and at the same time the Danish self-sufficiency could be sustained,” says Erling H. Stenby, Head of Department at DTU

Chemistry and member of the CERE faculty. Erling H. Stenby represents Denmark in the IEA cooperation on EOR.

Martin Rune Pedersen, Vice President for TOTAL’s activities in Denmark, Norway, and the Netherlands, adds:

“TOTAL remains fully committed to contribute to Danish self-sufficiency through continued development of the Danish North Sea. A part of this effort is technology investments that may raise the production rate in these complex fields. The effort takes place both internally in TOTAL, and in close cooperation with the Danish Hydrocarbon Research & Technology Center (DHRTC) as well as Danish and international universities and operators. This is part of our motivation for supporting international cooperation such as the IEA-EOR conference.”

An ongoing effort since 1972

Enhanced Oil Recovery is a key part of the national strategy “The future oil and gas sector in Denmark” from July 2017.

“The strategy presents estimates of the amounts of oil and gas expected to be

produced from known fields. 21 pct. of the known oil and gas has already been produced. According to industry estimates this percentage will reach 27 pct. If the technologies identified in the strategy can be developed further and implemented at commercial scale, it is estimated that production can be increased further to reach up to 34 pct. of the known oil and gas,” says Trine Sannem Mønsted, Head of Office at The Danish Energy Agency.

Martin Rune Pedersen, TOTAL, stresses that significant progress has already been made over the last few decades:

“As production commenced at the first Danish field, Dan, in 1972, it was expected that only a few percent of the oil could be produced. However, during the 1980’ies new technology such as long horizontal wells and water injection raised production levels considerably. In certain fields we see production rates above 30 percent today. We continue to focus at raising the level through water injection optimization and development of new cost-effective EOR methods such as gas injection and injection of sea water with modified salinity.”

International cooperation has helped Denmark

Denmark has taken part in the EOR cooperation in IEA since 1987. Participation in the EOR cooperation in IEA is almost cost-free. No secretariat is maintained, and no joint research schemes are funded. The main activity is exchange of experience.

“As a relatively small player within oil and gas, the participation has been of high value to Denmark,” says Erling H. Stenby. “Over the years, large fluctuations have been seen in the prospects for obtaining Danish public funding for oil and gas related research. Still, we have always remained up-to-date on the latest EOR trends through the IEA cooperation.”

For CERE, the cooperation has led to long term collaborations with a number of world leading research institutions including Stanford University (US), Imperial College (UK), and IFP Energies Nouvelles (France).

Erling H. Stenby
Professor



The IEA EOR Workshop & Symposium attracted leading researchers from all over the world. In addition to the strong scientific program the organizers had included several special treats for guests. This included a guided tour to the famous chalk outcrops at Stevns Klinter, a nice venue at Schæffergården close to DTU, and a very special dinner at the Carlsberg Academy with special beers otherwise not available to the public.”

Interview:

The World still craves Oil

Enhanced Oil Recovery continues to be highly relevant. Especially, the interest in polymer EOR is growing, while most other EOR techniques are operated at steady levels.

Despite renewable energy transition efforts in several countries, the world will remain dependent on oil and gas at least for the next decades.

“New large fields are rarely found, while substantial risks are involved around fields at ultradeep waters or in the Arctic region. Therefore, interest in being able to produce more from the existing fields has become very high,” explains Torsten Clemens, Chairman of the EOR Executive Committee under IEA.

Torsten Clemens is Chief Scientist for Reservoir Engineering at Austrian based energy corporation OMV, a long-standing member of the CERE industry Consortium.

“Admittedly, the status of Denmark as an oil exporting country surprised me, when I joined the work in IEA,” says Torsten Clemens. “Since, I have learned of the efforts carried out especially by Maersk Oil – now acquired by TOTAL. The carbonate reservoirs in the North Sea are really tight, and being able to produce them is truly impressive. Still, there seems to be a potential for producing even more with improved technology.”

Informal discussions are important

The annual IEA-EOR conferences allow the countries to obtain access to results from research activities and field trials which have often been highly costly and surrounded by some secrecy.

“Personal relations are important. Presenters at a conference will traditionally want to convey a nice image. But as a participant,

learning of the hardships and obstacles in the various field trials and other projects is also very valuable. This is the type of information, you may be able to get through informal discussions,” Torsten Clemens remarks.

The IEA conferences are a bit different from other conferences on EOR:

“In a traditional format, the presenters will be chosen by a committee based on abstracts. This often leads to some bias, as the committee will tend to favor groups from institutions and countries with a long track record of academic contributions. But in the IEA setup, the member countries choose who to send. This often leads to fresh new input – for instance from Mexico and Colombia. Both countries have joined the cooperation recently,” notes Torsten Clemens.

Another example is China.

“Not least in polymer EOR, China has been the leading country for many years now. Yet, Chinese presentations are quite rare at international conferences, but they always present here,” says Torsten Clemens.

Rising interest in polymer EOR

In recent years, polymer EOR has been taken up by a number of other nations besides China.

“For instance, by Oman, India, and Canada. Interest in polymer EOR is growing quite rapidly, while we see a steady situation for most other EOR techniques.”

Historically, steam injection was the first EOR technique to really catch on.

“In fact, you cannot produce a number of heavy oils without steam injection. Especially in the US, steam injection was believed to become very significant, but the successful results for production in shale have decreased the general demand for EOR in USA. Also, other EOR techniques like injection of nitrogen gas are at a relatively stable level.”

Another gas has gained special attention, namely CO₂. This is due to the fact, that CO₂ injection may not just be an EOR technique but also contribute to climate protection if the CO₂ stays underground.

“In principle, this is a very interesting technique. However, some issues around public acceptance remain unsolved. First and foremost, the costs of separating CO₂ from flue gas at power plants are currently too high for the technique to be fully viable.”

New EOR Scientific Framework

The Thermal EOR International Workshop, initiated by the Kazan Federal University, Russia, attracts still more participants.

CERE was strongly present as the Thermal EOR International Workshop in 2018 was held for the third time. Whereas the two previous events were both held in Russia, this time China played host.

“Although called a workshop, the event has actually developed into more of a conference, with more than 200 participants. Further, it has become more international,” says Senior Researcher Wei Yan, CERE.

Professor Erling H. Stenby, CERE, gave an invited plenary lecture providing an overview of the challenges in compositional simulation of thermal EOR processes, emphasizing CERE’s contributions to the field. Thermal EOR covers a variety of processes utilizing thermal energy to produce oil that is otherwise difficult to recover. Although thermal energy is usually the major driver, some sophisticated thermal EOR processes can involve other important mechanisms that must be addressed specifically. One such example is production of heavy oil with steam and solvent, which has gained increasing attention in recent years. Co-injection or alternating injection of solvent is proposed to reduce energy and water consumption or to handle reservoirs with thin pay zones and/or bottom water aquifers. Nevertheless, coexistence of steam, solvent and heavy oil at high temperatures



“The carbonate reservoirs in the North Sea are really tight, and being able to produce them is truly impressive.”

Torsten Clemens, Chairman of the EOR Executive Committee under IEA

creates a complicated multiple phases system, which must be described by a compositional model.

More than thermal EOR

Contributing to the decision of the CERE faculty members to participate, was the fact that the conference is widening its spectrum of disciplines.

“Overall, it is mostly specialized in thermal EOR but it is developing to become more inclusive. Actually, my own presentation at the conference had little to do with thermal EOR but was focused on gas injection modeling in shale,” notes Wei Yan.

Gas injection in shale requires an adequate description of the underlying phase behavior.

“However, we need to address some distinctive features of gas injection in shale in its modeling. Firstly, due to the nano-scale pore sizes of shale, the capillary pressure effects are more pronounced in phase equilibrium. Secondly, due to the high organic content, the adsorption effect is non-negligible. We have attempted to follow the classical approach for gas injection study in the gas injection modeling for shale, and

developed the tools for analysis at different levels,” explains Wei Yan.

From Kazan to Chengdu

The developed phase equilibrium calculation tools can robustly and efficiently calculate flash with strong capillary pressure and adsorption.

“We investigated how to account for pore size distribution in the modeling of capillary pressure and how to reasonably model multicomponent adsorption on shale. At the PVT modeling level, we developed a PVT software tool to simulate the classic experiments: constant mass expansion, differential liberation, and constant volume depletion in the presence of capillary pressure and adsorption. Thereby we can analyze the influence of capillary pressure and adsorption. We further integrated the flash module with capillary pressure and adsorption into a slim tube simulator to calculate the minimum miscibility pressure under the influence of capillary pressure and adsorption. Finally, at the simulation level, we included the capillary pressure in a compositional reservoir simulator to simulate the performance of gas injection in shale where the capillary pressure effects are considered,” says Wei Yan.

The thermal EOR workshop series was founded and initially organized by the Kazan Federal University, Russia. The third Thermal EOR International Workshop was held 15-19 October 2018 in Chengdu, China.

Oil and Gas Research at DTU

Enhanced Oil Recovery (EOR) is the term used for producing oil and gas with methods that are beyond water flooding and other standard methods. Among EOR techniques in everyday use globally are injection of steam, CO₂, and other gasses including nitrogen. A relatively new and rising trend is to inject small amounts of chemicals which cause the oil to detach from the surrounding rock surface. However, none of these techniques are currently applied in Denmark. The oil and gas related research at DTU is mainly done in two centers. The Center for Energy Resources Engineering (CERE) has an international focus and also include other applications besides oil and gas, while the Danish Hydrocarbon Research & Technology Center (DHRTC) is a national center focusing specifically at the Danish part of the North Sea. The two centers cooperate extensively.

NEWS from CERE

Chairman talks around the Globe

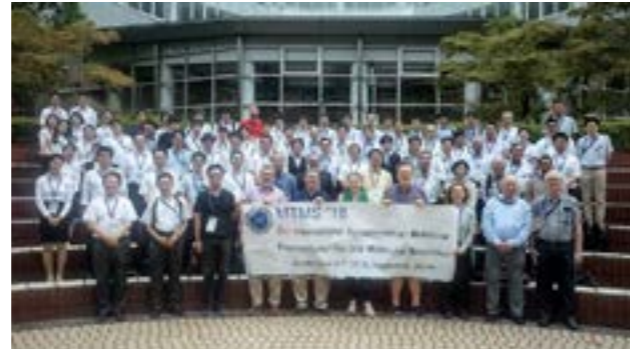
The past year has been busy for CERE Chairman, Georgios Kontogeorgis, in terms of invited lectures.

Perhaps most prominently, Professor Kontogeorgis was selected for the 2018 Distinguished Lecture in Thermodynamics by the Working Party on Thermodynamics within the European Federation of Chemical Engineering (EFCE). Under the title "Mysteries of Water Thermodynamics – Questions and some Answers" the lecture was delivered at the 30th European Symposium on Applied Thermodynamics in Prague, Czech Republic, June 10-13.

Soon after, Georgios Kontogeorgis attended the 8th International Symposium on Molecular Thermodynamic and Molecular Simulation (MTMS 18) in Narashino, Japan, September 4-7. Here, he gave an invited keynote lecture on electrolyte thermodynamics. The talk was based on a recently published manuscript in Fluid Phase Equilibria, co-authored with CERE faculty, Associate Professor Kaj Thomsen and

Dr. Bjørn Maribo-Mogensen. The manuscript is featured on the list of most downloaded articles of the journal in 2018.

Also, Professor Kontogeorgis contributed to a unique industry event, as AkzoNobel (now called Nouryon) organized a symposium in honor of the 25th work anniversary of Dr. Antoon ten Kate. The symposium has held at the corporation's research center in Deventer, The Netherlands, October 12. In his invited presentation, the CERE Chairman addressed "Thermodynamics for a Sustainable Chemical Engineering in a Changing World – a pragmatic view". AkzoNobel is a long-standing member of the CERE industry consortium.



Dr. Antoon ten Kate, Lead scientist, Nouryon

Finally, Latin America was visited, as Professor Kontogeorgis was invited to give the opening lecture at the 11th Iberoamerican Conference on Phase Equilibria and Fluid Properties for Process Design – or EQUIFASE for short. He chose "Advanced Equations of State – but how much have we advanced Science and Engineering?" as his topic. The EQUIFASE conference took place October 22-25 in Córdoba, Argentina.

New Territories in Biology

Nikolaj Sorgenfrei Blom, Senior Researcher at CERE, was invited to give the opening presentation at the "New Frontiers in Biology" meeting in Rome, Italy, on March 2, 2018. His talk "Genomics, Microbiomics and Water" bridged several frontier science fields and emphasized the courage needed in groundbreaking scientific discovery.



Postdoc Project on Smart Water

Associate Professor Alexander Shapiro, CERE, and Advisor Simon I. Andersen, Danish Hydrocarbon Research and Technology Centre (DHRTC), have been granted support from DHRTC for a Postdoc project on water flooding.

Known as "smart water", a strategy in oil production is to inject water with a modified composition with the purpose of extracting additional oil from a reservoir. Extraction of the residual oil from a petroleum reservoir by injection of a brine with a different salinity has long been considered promising. However, the exact mechanism of action remains unclear. It has been hypothesized that sharp variation of the salinity can help production.

The residual oil in a porous rock is found as separate drops surrounded by brine, and a moving front between brines of different salinity might be able to mobilize the oil drops.

A microfluidic experiment in the new project will aim to test this hypothesis. This should either disclose an important mechanism in smart water oil production or eliminate this mechanism from further consideration. The project has a duration of one year.



Tian Wang, Postdoc project on Smart Water

Strong Presence at Carbon Capture Conference

More than 900 participants for the 14th international conference on greenhouse gas technologies (GHGT 14) was a clear indication of the rising interest in limiting the global emissions of CO₂ and other greenhouse gases. CERE was represented by Associate Professors Nicolas von Solms and Philip L. Fosbøl, and Research Assistant Randi Neerup. They brought no less than 6 posters, and also contributed to international collaboration in 3 other oral presentations and posters. Their topics included results from the most recent collaborations with the Technology Center Mongstad in Norway, and the BioCO₂ project which included kinetics and pilot testing. CERE also presented hydrate swapping, bi-phasic solvents, and new processes principles for CO₂ capture. The GHGT 14 was held in Melbourne, Australia, October 21-26.



Foto by Max Klime

NEWS from CERE



Michael Bache, Senior Researcher at CERE

ExxonMobil Presentation on Vapor Solubility

The staff and students at CERE were able to gain new insight into modeling of vapor solubility in semi-crystalline polyethylene at December 12 when Dr. Brian Greenhalgh, researcher with ExxonMobil, Houston, USA, visited. Dr. Greenhalgh presented experience within theory and application of a thermodynamic model developed by himself and his colleague at ExxonMobil, Dr. Joseph Moebus.

In the gas phase polyethylene (GPPE) process, monomers react in a continuous fluidized bed of catalyst, producing solid polymer granules. The latest generation of the condensed-mode GPPE achieves enhanced cooling capacity through the use



of inert condensing agents. These are non-polymerizing species that vaporize in the reactor and condense in the cycle gas cooler. An example is isopentane.

The thermodynamic model developed by Greenhalgh and Moebus is based on an activity coefficient modification of the Sako-Wu-Prausnitz equation of state, and uses a polymer-specific parameter to describe the effect of crystalline polymer domains on vapor solubility.

Water Research yields Poster Award

Michael Bache, Senior Researcher at CERE, won first prize in the poster competition at the 13th international conference on the physics, chemistry and biology of water held in Sofia, Bulgaria, October 18-21.

The winning poster was entitled "Could a device used for CaCO₃ de-scaling change the properties of water itself?" Here, Michael Bache explains how he was approached by a Danish company, Amtech. The company markets an ultrasound-based device, which successfully removes CaCO₃ from tap water. "Everybody is happy, except the scientists – since we don't know why the device works," as Michael Bache stated in his oral presentation.

Through a series of highly advanced investigations – X-ray diffraction (XRD), Fourier Transformed Infra-Red (FT-IR), and Surface Enhanced Raman Spectroscopy – at various departments at DTU, the Senior Researcher arrived at the conclusion that the magnetic emissions from the device were able to induce changes to the properties of the water itself. The presentation can be heard at the website of the conference: www.waterconf.org

Workshop on Sustainable Fuels for Aviation

On 20 November 2018, Nordic Energy Research (NER), Nordic Initiative for Sustainable Aviation (NISA) and DTU organized a workshop at Nordens Hus in Copenhagen to explore policies, technology needs and market development. 60 people from the aviation industry (airline, fuel producers and airports), Nordic aviation administrators, and researchers shared their perspectives.

Director Hans Jørgen Koch, Nordic Energy Research, noted upon the conclusion of the workshop;

"The Nordic countries have a unique opportunity to become a beacon for the aviation industry in their quest to deliver on the Paris agreement. We have access to sustainable biomass, producers that are prepared to ramp up production, aviation

administrations and national governments determined to increase the mix of sustainable aviation fuel and also investigate new production routes, including electrification of short-range aviation."

CERE faculty member, Associate Professor Hariklia Gavala, coordinated the DTU contributions to the workshop.

Associate Professor Hariklia Gavala, DTU Chemical Engineering



In the Lab for 25 Years



With CERE as his main workplace, laboratory technician Zacharias Tecle was able to celebrate 25 years of service for the Danish state.



Targeting the Fourth Phase of Water

"Structured Water and its Implications for Biology, Chemistry and Physics" – WATERSTRUC for short – is a new multidisciplinary project at CERE. Supported by VILLUM FONDEN (part of the VELUX FOUNDATIONS), the project will look into fundamental properties of water.

Liquid water can form large self-organized structures around ions and particles as well as close to surfaces. Such structures are proposed to be an intermediate phase between liquid water and ice; in other words, a fourth phase of water.

A possible implication is that such structured water can act as a "water battery" producing electrical current, driven by infrared light. Among other questions addressed in WATERSTRUC is whether water itself can form macroscopic long-range liquid crystals.

The project is coordinated by Senior Researcher Johan Kronholm, CERE.

PhD

Sandstone in Energy Resources Engineering

Several geological properties are highly relevant to energy resources engineering. Knowledge of thermal conductivity, permeability, stiffness, and strength of the reservoir rock is key to successful and safe exploration of the deep High Pressure High Temperature (HPHT) petroleum reservoirs, and equally relevant in evaluating the potential of a geothermal reservoir. The project provides new knowledge about temperature effects on rock stiffness and rock strength in sandstone, as well as estimation of the temperature effect on downhole effective stress. Further, a new model for thermal conductivity in sandstone is presented.

As the petroleum industry targets deeply buried HPHT reservoirs, e.g. in the central North Sea, knowledge of temperature effects on the stiffness and strength of the reservoir rock becomes critical. The success and safety of drilling operations rely on accurate estimates of the subsurface effective stress field. Currently, such estimations will typically not include temperature effects. Limiting its scope to one of the relevant classes of sedimentary rock, sandstone, the project aims to change this picture.

Sandstone from three wells in the central North Sea Basin was studied. Samples collected from depths exceeding 5 km and in-situ temperatures above 170 °C were tested in the dry state at temperatures from ambient to in-situ. Results show a stiffening of the material for increasing test temperature. This can be attributed to thermal expansion of the constituting mineral particles. Likewise, strength parameters derived from measurements of shear failure at ambient

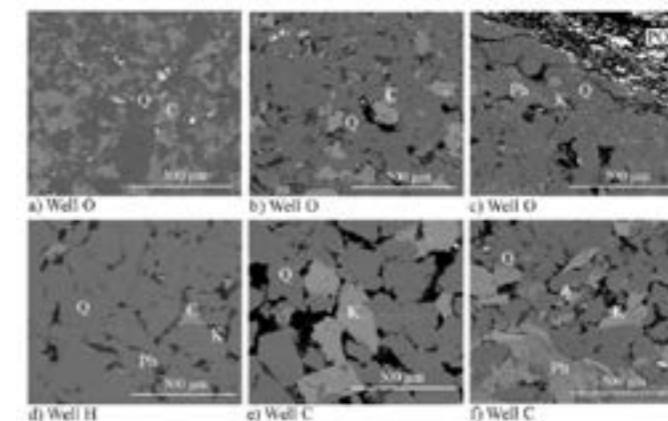
and in-situ temperature show strengthening with temperature, which may also be attributed to thermal expansion of constituting minerals.

HPHT reservoirs may not only be subject to high temperature and extreme stress-fields but also to high regional overpressure. The effective stress according to the classical Biot equation (Biot 1941) is a function of the total stress (subsurface overburden), but also of the magnitude of total stress carried by the pore fluid. Results from interpreting logging data by using the Biot equation indicate a neutral effective stress at great depth, so that the overburden load may be carried solely by the pore pressure.

Another property of high relevance to both petroleum and geothermal energy engineering is permeability. In the project, Nuclear Magnetic Resonance (NMR) spectroscopy experiments combined with Kozeny's equation showed that the largest pores in the sandstones do not form a continuous path, and consequently the smaller pores control the overall permeability.

Due to minimal subsurface coring, assessment of depth variations in thermal conductivity is typically limited to applying empirical relations to downhole logging data. However, by combining input parameters from the concepts of rock stiffness and permeability, it is possible to establish a new model for thermal conductivity. Provided a given mineralogical composition, the model can estimate formation thermal conductivity as a function of depth using solely parameters quantified through conventional

log interpretation. The applicability of the model was demonstrated by comparing measured data with model predictions.



BSEM-images of sandstone from well O, H and C, representing side-trim material from plugs. Q = quartz, C = calcite, K = feldspar, Ph = phyllosilicate, P = pyrite, PO = pyrite in organic matter.



Tobias Orlander, PhD.

Currently Postdoc in CERE, DTU Civil Engineering.

Full title: "Temperature and Porosity-elasticity of Sedimentary Rocks - Thermal Conductivity, Permeability and Temperature Effects on Stiffness and Strength Properties of Sandstones"

Supervisors
Ida L. Fabricius, Katrine Alling Andreassen.

Funded by DTU, Innovation Fund Denmark, Maersk Oil, and DONG Energy.

Scaling during deep Oil Exploration

The world's growing demand for energy has triggered interest in producing HPHT (high pressure high temperature) oil and gas reservoirs which are found at greater depth than conventional reservoirs. Several HPHT reserves are present in the Danish part of the North Sea. However, a number of challenges must be overcome in order to produce these fields in a safe and economically feasible way. The project investigates one such challenge: deposition of minerals, or scaling.

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 possibly causing production losses and even total stop of production.

HPHT conditions are highly corrosive, not least due to the presence of H_2S . While carbonates are the most common scaling materials in conventional oil and gas exploration, scaling of sulfides – mainly Zinc Sulfide (ZnS), Lead Sulfide (PbS), and Iron Sulfide (FeS) – is also seen under HPHT conditions. These types of scaling are problematic, not least since the sulfides are less affected by conventional inhibitors.

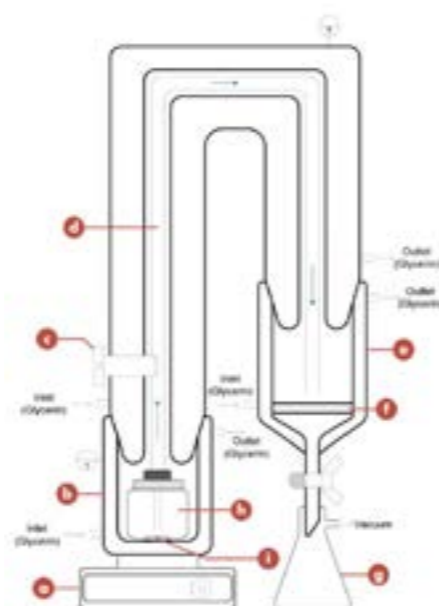
Compression of a fluid usually leads to an increase in temperature. This phenomenon is known as the Joule-Thomson Effect (JTE). An inversion of this effect can take place at extreme conditions, resulting in temperature increase during decompression. It was feared that in relation to HPHT fields, decompression could result in a temperature increase so large that water would evaporate and the salt dissolved in water would precipitate and block the pipes. In this project, JTE and its inversion were evaluated to determine the impact of the decompression process on the final temperature of a confined fluid – either water, oil, or brine – at HPHT conditions. The increase of temperature for oil at non-isenthalpic conditions was established as 7.4 °C. This represents a reduction of 16.8 °C compared to the final temperature estimated at isenthalpic conditions, and shows that if JTE is estimated at isenthalpic conditions, the final temperature is overestimated.

An important part of the project was the design of an experimental apparatus. Further, to develop a reliable experimental methodology for measuring the solubility of minerals at HPHT conditions. A borosilicate glass set-up was chosen for measuring the solubility at temperatures up to 80 °C. Additionally, a High-Temperature Cell made of Titanium was built to perform solubility experiments at up to 200 °C and 60 bars. The set-up has mainly three advantages. Firstly, anoxic conditions are guaranteed throughout the process. Secondly, sufficiently long contact time was assured between the solvent and the solute to assure steady state conditions. And thirdly, an adequate analytical technique for measuring trace elements was chosen – namely Inductively Coupled Plasma Optical Emission Spectrometry (ICP-OES).

The experimental data were used for adjusting the Extended UNIQUAC model to predict the solubility of sulfides by means of thermodynamic calculations. According to the results, the model can represent the solid-liquid equilibrium of ZnS and FeS up to 100 °C. Difficulties were encountered for representing the solid-liquid equilibrium of the PbS aqueous system. The inclusion of complexes into the speciation equilibrium model is required to achieve good results.

In conclusion, the project contributes to better understanding of the behavior of sulfide scaling materials at HPHT conditions, and may hopefully assist operators in addressing scaling challenges in the future.

Experimental set-up for measurements of ZnS. (a) Stirring plate, (b) equilibration cell, (c) Teflon screw, (d) transport of sample at constant temperature, (e) filter chamber, (f) porous body, (g) side-arm flask, (h) vial and (i) stirring bar.



Diana Carolina Figueroa Murcia, PhD.

Currently Postdoc in CERE, DTU Chemical Engineering.

Full title: "High Pressure High Temperature Reservoir Fluids with Focus on Scaling and Thermodynamic Modeling."

Supervisors
Kaj Thomsen,
Philip L. Fosbøl.

The project was a part of the Next Oil Project funded by Maersk Oil, DONG Energy, and Innovation Fund Denmark.

Pipelines for CO₂ Transport in Deep Waters

Pipelines for CO₂ Transport in Deep Waters Injection of CO₂ is a promising technique for Enhanced Oil Recovery. It is an intrinsic advantage that the CO₂ can be stored in the reservoir, limiting the release into the atmosphere of this greenhouse gas. However, an often-overlooked challenge is transportation of CO₂. The project investigates several critical parameters for polymers that are needed in pipelines for the purpose.

Offshore oil exploration continues to move into deeper reservoirs and larger water depths leading to extreme conditions, not least to high levels of pressure. These conditions challenge pipeline technology.

For some years, the trend in offshore exploration has been to prefer flexible pipelines which are faster and safer to install than rigid pipelines. A flexible pipeline consists of several layers of materials, including polymeric layers. The layer under study in this project is the inner polymeric layer, which needs to have chemical and mechanical compatibility with the fluid being transported. Under deep water conditions, CO₂ is likely to be in the supercritical state. Despite being non-toxic and non-flammable, the interaction of supercritical CO₂ with the inner polymer layer may challenge pipeline stability. Firstly, the CO₂ may cause swelling of the polymer leading to ruptures, and secondly gradual degradation of the polymer, resulting in loss of key barrier properties.

Currently, three types of polymers are used for the inner layer: poly(vinylidene fluoride) (PVDF), crosslinked polyethylene (XLPE), and polyamide 11 (PA11).

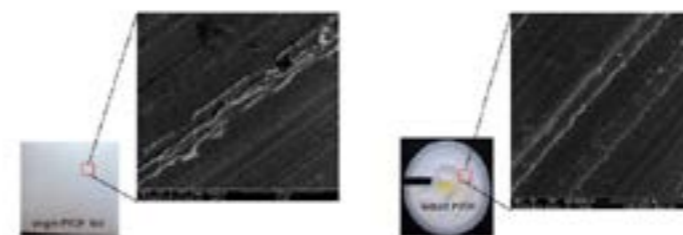
In the project, the solubility of pure CO₂ was measured for XLPE and PVDF for temperatures up

to 403 K and pressures up to 300 bar. It was observed that the solubility temperature dependence followed the Arrhenius equation, decaying with temperature increase. The solubility increased with temperature. The solubility was modelled with the sPC-SAFT equation of state, which was able to correlate to the experimental data, although a temperature dependent, binary interaction parameter was required.

Polymer swelling was seen to increase with temperature for PVDF and decrease for XLPE; this difference might be due to the very high degree of crosslinking in XLPE.

The permeability of gas was measured at up to 345 bar and 403 K for PVDF, and up to 650 bar and 403 K for XLPE and PA11. It was shown, that the permeability always increases with increasing temperature, while the permeability increases with pressure for PVDF and PA11 and decreases with pressure for XLPE. This is explained by the contrary effects of pressure on the free-volume, which may decrease because of the increase in the polymer density, or increase due to the penetrant increase that can lead to plasticization of the polymeric chains. The only plasticized polymer studied, PA11, showed a 2.58 % loss in weight from pre- to post-test. As the effect is not seen in the two other polymers, it is assumed that the plasticizer is being removed.

Finally, diffusion was calculated. The diffusion was shown to have a more pronounced effect in the permeability than the solubility with respect to both temperature and pressure. With increasing pressure, diffusion increases in PVDF and increases in XLPE, while solubility increases in both polymers. The permeability shows the same pressure behavior as diffusion, opposite to the solubility.



SEM images of PVDF, before and after, permeability tests conducted at 650 bar and 318 K with a mixture composed by 90 mol% CO₂ and 10 mol% CH₄.



Susana Raquel Melo de Almeida, PhD.

Currently Postdoc at CERE, DTU Chemical Engineering.

Full title: "Measurement and Modelling of Gas Permeability and Solubility in Polymers for Offshore Pipelines."

Supervisors
Nicolas von Solms,
Georgios Kontogeorgis.

The project was funded by National Oilwell Varco (NOV) and DTU Chemical Engineering.

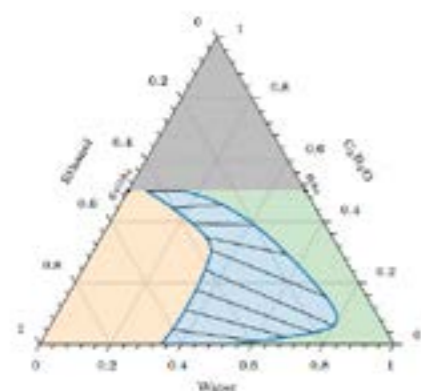
Better Calculation of Chemical and Phase Equilibria

Simultaneous calculation of chemical and phase equilibria (CPE) is highly relevant in the chemical industry, in oil and gas production, and in geochemistry. The project presents a new set of algorithms which are demonstrated to be robust and effective even for complicated systems.

CPE calculations are essential in demanding simulations of industrial processes. The applications include reactive distillation, heterogeneous organic synthesis, fuel synthesis from renewable feedstocks, and oil and gas production. Such calculations are also useful in association equation of state models, since association can be regarded as a type of reaction.

One class of CPE methods are the stoichiometric. While these are more intuitive, they are known to be less effective for systems involving many reactions. As complex challenges are the focus of this project, a non-stoichiometric approach was thus chosen.

The proposed solution is a hybrid of two different non-stoichiometric approaches and is therefore named "the combined method" here. In the first of the two methods, the Lagrange multipliers method, successive substitution is employed to solve a modified set of equations originating from the Lagrangian conditions at the minimum. In the second method, the modified RAND method, one of the Lagrangian conditions is linearized around the current estimate of mole numbers. Composition derivatives of fugacity or activity coefficients are utilized to achieve quadratic convergence.



Ternary diagram of elements in acetic acid/ethanol esterification at 355 K and 1 atm (binodal curve (—), tie lines (---), VLE region (blue), vapor region (orange), liquid region (green), infeasible region (grey), HAc (acetic acid), EtOAc (ethyl acetate)).

Combining the two methods improves robustness and efficiency. The Lagrange multipliers method is used for the first iterations of successive substitution, and the modified RAND method for final second-order convergence. The combined algorithm has several advantages including a smaller system of equations (fewer variables), less sensitivity to initial estimates, the same treatment for all components and all phases, and the ability to monitor the decrease in Gibbs energy in the modified RAND step to guide convergence.

The combined method was applied to vapor-liquid, liquid-liquid, and vapor-liquid-liquid equilibrium of ideal as well as non-ideal systems for acid/alcohol esterifications, alkene/alcohol etherifications, hydration, hydrogenation, and isomer preparation. Additionally, predictions were made for the more complex transesterification of two individual triglycerides with methanol, which entails five chemical reactions and can result in one-, two-, or even three-phase equilibrium. Finally, CPE calculations were attempted for electrolyte systems, and the equilibrium solution was obtained for aqueous mixtures of electrolytes in contact with a vapor and a solid phase. As the method is robust to the presence of a solid phase, the algorithms are applicable even to more complicated geological systems with an electrolyte aqueous phase and multiple solids.

In summary, the method proved applicable all the way from simple one-reaction ideal systems to highly non-ideal electrolyte mixtures with speciation reactions and solids. Both algorithms were able to converge to the equilibrium solutions. Considering CPU time and the reasonable number of iterations, the method is demonstrated to be efficient and robust.

The project also involved a small study on dimethyl ether (DME) phase equilibrium modeling.



Christos Tsanas, PhD

Currently Postdoc at CERE, DTU Chemistry.

Full title: "Simultaneous Chemical and Phase Equilibrium Calculations with Non-stoichiometric Methods".

Supervisors
Wei Yan,
Erling H. Stenby.

Funded by DTU Chemistry, Co-sponsored by the Danish Hydrocarbon Research and Technology Centre (DHRTC).

Optimization of Production over Oilfields

Oil production most often involves multiple injection and production wells across the same oilfield, and the interaction between these wells can be complex. Thus, the chosen production strategy will have a significant impact on the profitability over the total life time of the field. To manually devise the optimal strategy is non-trivial and time-consuming. Instead, the project has developed computer-based methods for the task.

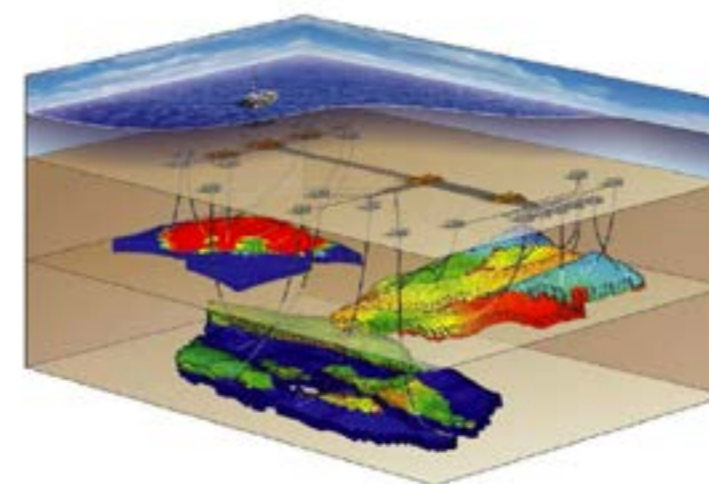
Nonlinear model predictive control (NMPC) is a cost-effective approach for improving the use of the various recovery techniques, including water flooding, enhanced oil recovery etc. The project investigates a NMPC strategy aimed at optimizing the total oil recovery measured as the net present value over the life time of the reservoir. Oil reservoir management based on NMPC is an example of closed-loop reservoir management (CLRM). Here, data assimilation (e.g. history matching) is combined with model-based optimization.

NMPC algorithms compute closed-loop feedback control strategies by using the moving horizon optimization principle, i.e. by repeatedly solving dynamic optimization problems. Only the first part of the strategy is implemented in practice before a new strategy is computed based on new process measurements. This approach involves dynamical constraints, i.e. differential equations which represent a model of the process and describe the temporal evolution of a set of state variables.

In the project, the involved phase equilibrium problems are formulated as equality constrained optimization problems and the phase equilibrium conditions as the first order optimality conditions. Consequently, the phase equilibrium conditions are a set of algebraic equations. The conservation equations are a set of coupled partial differential equations. The method of lines is used to solve these partial differential-algebraic equations, and the partial differential equations are discretized with a finite volume method. The result is a set of differential equations, and combined with the phase equilibrium conditions, the model equations are a set of differential-algebraic equations (DAEs).

The project presents algorithms for simulation, state estimation, dynamic optimization, and NMPC of DAEs. A major deliverable from the project is an open-source thermodynamic software library called ThermoLib (available at www.psetools.org). ThermoLib provides Matlab and C routines for evaluating the enthalpy, entropy, and volume of ideal gas mixtures, ideal liquid mixtures, and non-ideal mixtures as functions of temperature, pressure, and mixed composition (in moles). All other thermodynamic functions can be computed from the enthalpy, entropy, and volume using fundamental thermodynamic relations.

The main novelty of the ThermoLib is that its routines also evaluate the first and second order derivatives of the thermodynamic functions with respect to the temperature, pressure, and composition. The expressions for these derivatives are derived analytically.



An illustration of offshore oil production facilities. The colors illustrate the heterogeneity of the petrophysical properties of the reservoir rock (e.g. the porosity or the permeability). This figure originally appeared in Völcker, C. (2011). Production optimization of oil reservoirs. PhD thesis, Technical University of Denmark.



Tobias Kasper Skovborg Ritschel, PhD.

Currently with Z-Control.

Full title: "Nonlinear Model Predictive Control for Oil Reservoirs".

Supervisors:
John Bagterp Jørgensen,
Andrea Capolei.

Funded by:
The OPTION project.

Thermodynamic Models for Complex Systems

Exploration of unconventional reservoirs and the use of near-critical and super-critical fluids in separation processes are examples of the increasing complexity facing the oil and gas industry. Feasible implementation of the processes involved requires accurate knowledge of the thermophysical properties of the systems. Here, experimental measurements remain important but are also time-consuming and expensive. The project contributes to the further development of theoretical thermodynamic models which can supplement the experimental campaigns.

A known limitation of the classical thermodynamic models is the incorrect description of the behavior of fluids close to the critical point. In this region, the properties of the system are modified due to the strong fluctuations related to the long-range correlations between the molecules. Classic equations of state like Soave-Redlich-Kwong (SRK) and Cubic Plus Association (CPA), are based on mean-field theory, in which an average interaction potential is assumed for the particles. Therefore, they do not account for these long-range fluctuations.

In the project, incorporation of the long-range fluctuations into SRK and CPA was achieved using a recursive procedure developed by White and co-workers, following the renormalization group (RG) treatment proposed by Wilson. The method consists of a set of recursive relations where the fluctuations with respect to the density are considered in several iterations. The resulting model is non-analytical / asymptotic close to the critical point, but reduces to the traditional equation far from the critical region.

In addition to SRK and CPA, the non-mean-field equations were compared with the Patel-Teja (PT) equation of state. The results indicate that only the crossover equations were able to describe both the saturated and critical properties with high accuracy for non-associating and associating species.

Afterwards, the calculations were

extended to binary and ternary mixtures. Several groups of systems containing n-alkanes, n-alkanols, and carbon dioxide were studied. This allows for evaluation of the models to represent the different phase type behaviors observed in some homolog series, e.g. methane/n-alkane. Additionally, the comparison with experimental data showed the importance of the renormalization group corrections for the precise description of the volumetric properties of mixtures of non-associating components in near-critical regions.

For systems with hydrogen bonding components, the incorporation of density fluctuations in the classic models proved even more crucial. This is due to the fact that the overestimation of the critical properties with CPA is higher for associating components, which affects the representation of the phase behavior of mixtures, and cannot be corrected with the use of binary interaction parameters. On the other hand, the classic cubic models cannot represent the behavior of such systems, because they do not account for the formation of hydrogen bonds in the fluid.

In conclusion, the project has shown that the utilization of the recursive procedure based on RG theory corrects the behavior of the classic models near the critical point, thus becoming a relevant and useful tool for engineering applications, which include the design of equipment and control of the operation of complex processes.



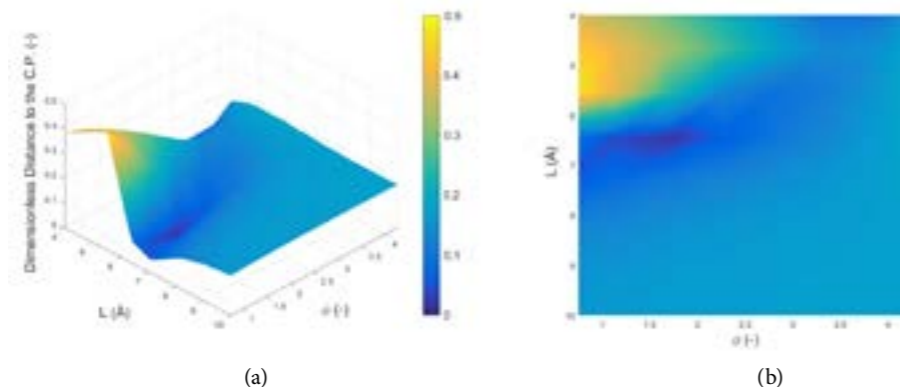
Andre Pinto Coelho Moniz Vinhal, PhD.

Currently Calsep.

Full title:
"Application of Advanced Thermodynamic Models in the Representation of the Global Phase Behavior of Fluids of Interest in the Oil & Gas Industry."

Supervisors
Georgios Kontogeorgis, Wei Yan.

Funded by
The Brazilian National Council for Scientific and Technological Development.



Dimensionless distance to the critical point as a function of the parameters of the recursive procedure in the CCPA for n-pentane.

Conference contributions & Invited speakers

JANUARY

33rd Nordic Geological Winter Meeting, Technical University of Denmark (DTU), Kgs. Lyngby, Copenhagen, Denmark, 10-12 January 2018

L.T.P. Meireles, E.M. Storebø, I.L. Fabricius, "Impact of electrostatic forces on sediment porosity", 33rd Nordic Geological Winter Meeting, Technical University of Denmark (DTU), Kgs. Lyngby, Copenhagen, Denmark, 10-12 January 2018 (Poster)

T. Orlander, K.A. Andreassen, I.L. Fabricius, "Stiffening effect from temperature and stress on sandstones from the deep North Sea Basin", 33rd Nordic Geological Winter Meeting, Technical University of Denmark (DTU), Kgs. Lyngby, Copenhagen, Denmark, 10-12 January 2018 (Oral)

L. Paci, I. Rocchi, I.L. Fabricius, "Elastic moduli, stiffness and effective stress of chalk from Zealand (Denmark) and from Dan field (North Sea)", 33rd Nordic Geological Winter Meeting, Technical University of Denmark (DTU), Kgs. Lyngby, Copenhagen, Denmark, 10-12 January 2018 (Oral)

Thomas Guldborg Petersen, "Evidence of post-breakup tectonism on the Northeast Greenland shelf: Implications for "passive" margin conditions", 33rd Nordic Geological Winter Meeting, Technical University of Denmark (DTU), Kgs. Lyngby, Copenhagen, Denmark, 10-12 January 2018 (Oral)

FEBRUARY

SPE International Conference and Exhibition on Formation Damage Control, Louisiana, USA, 7-9 February 2018

Jyoti S Pandey, Negar Nazari, Kaj Thomsen, Reza Barati, "A Novel Equipment friendly and environment friendly well stimulation fluid for carbonate reservoir: Better Wormholes and Lower Corrosion at Reservoir Condition", SPE International

Conference and Exhibition on Formation Damage Control, Louisiana, USA, 7-9 February, 2018 (Oral)

MARCH

Frontiers in Biology, International meeting of the National Society of Biology, Rome, Italy, 2 March 2018

Nikolaj Sorgenfrei Blom, "Genomics, Microbiomics and Water – a Matrix of Life?", Frontiers in Biology, International meeting of the National Society of Biology, Rome, Italy, 2 March 2018 (invited speaker)

DANSIS seminar day on High order discretisation methods in CFD, Aarhus, Denmark, 21 March 2018

A.P. Engsig-Karup, "How to innovate using applied and computational mathematics – on bridging research in modern scientific computing paradigms with industrial applications", DANSIS seminar day on High order discretisation methods in CFD, Aarhus, Denmark, 21 March 2018 (Invited speaker)

MAY

26th European Biomass Conference & Exhibition, (EUBCE) Copenhagen, Denmark, 14-18 May 2018

A. Grimalt-Alemany, I.V. Skiadas, H.N. Gavala, "Syngas fermentation by mixed microbial consortia: enrichment and continuous fermentation", 26th European Biomass Conference & Exhibition, (EUBCE) Copenhagen, Denmark, 14-18 May 2018 (poster)

A. Burniol-Figols, C. Varrone, A.E. Daugaard, I.V. Skiadas, H.N. Gavala, "Combined production of polyhydroxyalkanoates (PHA) and 1,3-propanediol production from crude glycerol", 26th European Biomass Conference & Exhibition,

EUBCE 2018, Copenhagen, 14-18 May 2018 (Poster)

M. Torli, G. Kontogeorgis, P. L. Fosbøl, "Simulations and Thermodynamics for Recovery of Liquid Biofuels from Syngas Fermentation Processes", 26th European Biomass Conference & Exhibition, (EUBCE) Copenhagen, Denmark, 14-18 May 2018 (poster)

1st International Workshop on Marine Hydrodynamics Modelling, Harbin, China, 21-25 May 2018

A.P. Engsig-Karup, "High-order Accurate Fully Nonlinear Potential Flow Time-Domain Methods for Marine Hydrodynamics", 1st International Workshop on Marine Hydrodynamics Modelling, Harbin, China, 21-25 May 2018 (Invited speaker)

3rd IFAC Workshop on Automatic Control in Offshore Oil and Gas Production, Esbjerg, Denmark, 30 May-1 June 2018

T.K.S. Ritschel, J.B. Jørgensen, "Production Optimization of a Rigorous Thermal and Compositional Reservoir Flow model", 3rd IFAC Workshop on Automatic Control in Offshore Oil and Gas Production, Esbjerg, Denmark, 30 May-1 June 2018 (oral) - Published in IFAC-PapersOnLine (proceedings) on ScienceDirect: <https://www.sciencedirect.com/science/article/pii/S2405896318306888?via%3Dihub>

T.K.S. Ritschel, J.B. Jørgensen, "Computation of Phase Equilibrium in Reservoir Simulation and Optimization", 3rd IFAC Workshop on Automatic Control in Offshore Oil and Gas Production, Esbjerg, Denmark, 30 May-1 June 2018 (oral) - Published in IFAC-PapersOnLine (proceedings) on ScienceDirect: <https://www.sciencedirect.com/science/article/pii/S2405896318306918?via%3Dihub>

T.K.S. Ritschel, J.B. Jørgensen, "The Extended Kalman Filter for State Estimation of Dynamic UV Flash Processes",

3rd IFAC Workshop on Automatic Control in Offshore Oil and Gas Production, Esbjerg, Denmark, 30 May-1 June 2018 (oral) - Published in IFAC-PapersOnLine (proceedings) on ScienceDirect: <https://www.sciencedirect.com/science/article/pii/S240589631830702X?via%3Dihub>

JUNE

DHRTC Young Researcher Day 2018, Kgs. Lyngby, Denmark, 8 June 2018

Jyoti S. Pandey, Nicolas von Solms, “Cavity Driven Acid Placement and Wormhole Propagation in Chalk Reservoir: Deeper Acid Penetration and Efficient Jetting. DHRTC Young Researcher Day 2018, Kgs. Lyngby, Denmark, 8 June 2018 (Poster)

30th European Symposium on Applied Thermodynamics (ESAT), Prague, Czech Republic, 10-13 June 2018

L. Sun, X. Liang, N. von Solms, G.M. Kontogeorgis, “Modeling Tetra-n-butyl Ammonium Halides Aqueous Solutions with the Electrolyte CPA Equation of State”, 30th European Symposium on Applied Thermodynamics (ESAT), Prague, Czech Republic, 10-13 June 2018 (oral)

Georgios M. Kontogeorgis, “Mysteries of Water Thermodynamics – Questions and some Answers”, 30th European Symposium on Applied Thermodynamics (ESAT), Prague, Czech Republic, 10-13 June 2018 (Invited Plenary talk in connection to “Excellence Award in Applied Thermodynamics – distinguished lecture”, June 2018 Awarded from European Federation of Chemical Engineering)

T. Regueira, M-L. Glykioti, N. Kottaki, Y. Liu, E. H. Stenby, W. Yan, “Extended PVT study of high pressure-high temperature reservoir fluids including the reverse Joule-Thomson effect”, 30th European Symposium on Applied Thermodynamics (ESAT), Prague, Czech Republic, 10-13 June 2018 (oral)

E.L. Camacho Vergara, G.M. Kontogeorgis, X. Liang, “Adsorption and Interfacial Tension of Inhomogeneous Fluids with Classical Density Functional Theory Approaches”, 30th European Symposium on Applied Thermodynamics (ESAT), Prague, Czech Republic, 10-13 June 2018 (poster)

F.J. Kruger, G.M. Kontogeorgis, N. von Solms, “Phase equilibrium measurements and modelling of glycol + water + natural gas systems for the design of subsea dehydration units”, 30th European Symposium on Applied Thermodynamics (ESAT), Prague, Czech Republic, 10-13 June 2018 (oral)

D.R. Sandoval, M.L. Michelsen, W. Yan, E.H. Stenby, “Phase envelope in the presence of capillary pressure calculated using volume-based thermodynamics”, 30th European Symposium on Applied Thermodynamics (ESAT), Prague, Czech Republic, 10-13 June 2018 (Oral)

C. Tsanas, E. H. Stenby, W. Yan, “Calculation of multiphase chemical equilibrium in electrolyte solutions with non-stoichiometric methods”, 30th European Symposium on Applied Thermodynamics, (ESAT), Prague, Czech Republic, 10-13 June 2018 (oral)

C. Tsanas, E. H. Stenby, W. Yan, “Modeling of dimethyl ether partitioning for dimethyl ether enhanced waterflood processes”, 30th European Symposium on Applied Thermodynamics, (ESAT), Prague, Czech Republic, 10-13 June 2018 (poster)

Y.Q. Liu, T. Regueira, E. H. Stenby, W. Yan, “Experimental study of high pressure density and viscosity of asymmetric mixtures related to reservoir fluids”, 30th European Symposium on Applied Thermodynamics (ESAT), Prague, Czech Republic, 10-13 June 2018 (poster)

D. Paterson, E.H. Stenby, W. Yan, “Use of Natural Variables to Solve State Function Based Flash Problems”, 30th European Symposium on Applied Thermodynamics

(ESAT), Prague, Czech Republic, 10-13 June 2018 (poster)

D. Paterson, M.L. Michelsen, E.H. Stenby, W. Yan, “Use of (T,V) Variables to Rapidly Solve Isothermal Flash Problems for Complex Equations of State in Dynamic Simulation”, 30th European Symposium on Applied Thermodynamics (ESAT), Prague, Czech Republic, 10-13 June 2018 (poster)

28th The International Society of Offshore and Polar Engineers (ISOPE) 2018, Sapporo, Japan, 10-15 June 2018

A.P. Engsig-Karup, C. Eskilsson, “Spectral Element FNP Simulation of Focused Wave Groups Impacting a Fixed FPSO”, 28th The International Society of Offshore and Polar Engineers (ISOPE) 2018, Sapporo, Japan, 10-15 June 2018 (Invited speaker)

SPE EUROPEC featured at 80th EAGE Conference and Exhibition, Copenhagen, Denmark, 11-14 June 2018

T. Orlander, K.A. Andreassen, I.L. Fabricius, “Stiffening and strengthening by increased temperature of dry sandstones from the deep North Sea Basin”, SPE Europec featured at 80th EAGE Conference and Exhibition, Copenhagen, Denmark, 11-14 June 2018 (e-poster)

I. Orozova-Bekkevold, “The Overburden – the long neglected Cinderella”, SPE Europec featured at 80th EAGE Conference and Exhibition, Copenhagen, Denmark, 11-14 June 2018 (oral)

Wael Al-Masri, Christos Papaspyrou, Alexander Shapiro, Vural Suicmez, “Study of the Feasibility of the Carbon Dioxide Injection in a North Sea Petroleum Reservoir”, SPE Europec featured at 80th EAGE Conference and Exhibition, Copenhagen, Denmark, 11-14 June 2018 (oral)

M.W. Arshad, K.L. Feilberg, A. Shapiro, K. Thomsen. “Modified Brine Salinity and Nanoparticles Size-Dependent Emulsion

Formation in Enhanced Oil Recovery”, 80th EAGE Conference and Exhibition 2018, Copenhagen, Denmark, 11-14 June 2018 (Oral) - DOI: <https://doi.org/10.3997/2214-4609.201800757>

37th International Conference on Ocean, Offshore and Arctic Engineering (OMAE) 2018, Madrid, Spain, June 17-22 2018

D. Koukounas, C. Eskilsson, A.P. Engsig-Karup, A.P., “Numerical simulation of Peregrine breathers using a spectral element model”, 37th International Conference on Ocean, Offshore and Arctic Engineering (OMAE) 2018, Madrid, Spain, June 17-22 2018 (oral)

C. Monteserin, A.P. Engsig-Karup, C. Eskilsson, “Nonlinear Wave-body interaction using a mixed-eulerian-lagrangian spectral element model”, 37th International Conference on Ocean, Offshore and Arctic Engineering (OMAE) 2018, Madrid, Spain, June 17-22 2018 (oral)

JULY

The 19th International Conference on Petroleum Phase Behavior & Fouling, PetroPhase 2018, Park City, Utah, USA, 8-12 July 2018

F.J. Kruger, G.M. Kontogeorgis, N. von Solms, “Phase equilibrium measurements and modelling of glycol + water + natural gas systems for the design of subsea dehydration units”, The 19th International Conference on Petroleum Phase Behavior & Fouling, PetroPhase 2018, Park City, Utah, USA, 8-12 July 2018 (poster)

18th International Symposium on Solubility Phenomena and Related Thermodynamic Properties (ISSP-18), Tours, France, 15-20 July 2018

D.C. Figueroa-Murcia, P.L. Fosbøl, K. Thomsen, “Solubility measurements of zinc sulfide using a novel high temperature

titanium cell”, 18th International Symposium on Solubility Phenomena and Related Thermodynamic Properties (ISSP-18), Tours, France, 15-20 July 2018 (poster)

D.C. Figueroa-Murcia, P.L. Fosbøl, K. Thomsen, “Solubility measurements of zinc sulfide using a novel high temperature titanium cell”, 18th International Symposium on Solubility Phenomena and Related Thermodynamic Properties (ISSP-18), Tours, France, 15-20 July 2018 (oral)

K. Thomsen, “The solubility of struvite-k experimental measurement and modeling”, 18th International Symposium on Solubility Phenomena and Related Thermodynamic Properties (ISSP-18), Tours, France, 15-20 July 2018 (oral)

7th International Conference on Engineering for Waste and Biomass Valorization, Prague, Czech Republic, 2-5 July 2018

A. Grimalt-Alemany, I.V. Skiadas and H.N. Gavala, “Mixed culture biotechnology for biofuels production in syngas fermentation processes”, WasteEng2018, Prague, 2-5 July 2018 (oral)

36th International Conference for Coastal Engineering, Baltimore, Maryland, USA, 30 July-3 August 2018

U. Bosi, A.P. Engsig-Karup, C. Eskilsson, M. Ricchiuto, E. Sola, “A High-Order Spectral Element Unified Boussinesq Model for Floating Point Absorbers”, 36th International Conference for Coastal Engineering, Baltimore, Maryland, USA, 30 July-3 August 2018 (oral)

AUGUST

CINEMAX IV PhD Summer School, Toreby, Lolland, Denmark, 27-31 August, 2018

Jyoti S Pandey, Alexander S Shapiro, Nicolas von Solms, “Molecular Level

study of Methane Gas Production by Hydrate swapping using X Ray Computer Tomography”, CINEMAX IV PhD Summer School, Toreby, Lolland, Denmark 27-31 August 2018 (Abstract)

2nd IEEE Conference on Control Technology and Applications, Copenhagen, Denmark, August 21-24 2018

T.K.S. Ritschel, J.B. Jørgensen, “Nonlinear Filters for State Estimation of UV Flash Processes”, 2nd IEEE Conference on Control Technology and Applications, Copenhagen, Denmark, August 21-24 2018 (oral) - Published on IEEE Xplore: <https://ieeexplore.ieee.org/document/8511532>

SEPTEMBER

16th - European Conference on the Mathematics of Oil Recovery, ECMOR 2018, Barcelona, Spain, 3-6 September 2018

D.R. Sandoval, W. Yan, E.H. Stenby, “Compositional Simulation with Capillary Pressure for Oil Production from Tight Formation”, 16th European Conference on the Mathematics of Oil Recovery, ECMOR 2018, Barcelona, Spain, 3-6 September 2018 (Oral)

T.K.S. Ritschel, J.B. Jørgensen, “Production Optimization of Thermodynamically Rigorous Isothermal and Compositional Models”, 16th European Conference on the Mathematics of Oil Recovery, Barcelona, Spain, September 3-6 2018 (oral) - Published on EarthDoc: <http://www.earthdoc.org/publication/publicationdetails/?publication=93859>

D. Paterson, M.L. Michelsen, E.H. Stenby, W. Yan, “Compositional Reservoir Simulation Using (T,V) Variables Based Flash Calculation”, 16th European Conference on the Mathematics of Oil Recovery, ECMOR 2018, Barcelona, Spain, 3-6 September 2018 (oral)

39th IEA-EOR TCP Workshop and Symposium, Copenhagen, Denmark 3-7 September 2018

D. Paterson, E.H. Stenby, W. Yan, “Compositional modeling for thermal EOR simulation, 39th IEA-EOR TCP Workshop and Symposium, Copenhagen, Denmark 3-7 September 2018 (Oral)

D. Sandoval, E.H. Stenby, W. Yan, “Gas injection modeling in shale”, 39th IEA-EOR TCP Workshop and Symposium, Copenhagen, Denmark 3-7 September 2018 (Oral)

8th International Symposium on Molecular Thermodynamic and Molecular Simulation (MTMS 18), Narashino, Japan, 4-7 September 2018

Georgios M. Kontogeorgis, “Current Status and Challenges in Electrolyte Thermodynamics”, 8th International Symposium on Molecular Thermodynamic and Molecular Simulation (MTMS 18), Narashino, Japan, 4-7 September 2018 (Invited Keynote lecture)

Engineering in Chalk, London, United Kingdom, 17-18 September 2018

L.T.P. Meireles, C. Ravnås, M.J. Welch, I.L. Fabricius, “Failure characterization in geomechanical testing using Nuclear Magnetic Resonance spectroscopy”, Engineering in Chalk, London, United Kingdom, 17-18 September 2018 (oral)

L.P. Meireles, E.M. Storebø, M.J. Welch, I.L. Fabricius, “Investigation of controlling parameters on geomechanical properties of the Southern Danish Central Graben chalk”, Engineering in Chalk, London, United Kingdom, September 17-18 2018 (oral)

International Symposium on Energy Geotechnics SEG-2018, Lausanne, Switzerland, 25-28 September 2018

T. Orlander, L. Pasquinelli, I.L. Fabricius, “Using Biot’s coefficient in estimation of thermal conductivity of sandstones, paper, oral presentation”, International Symposium on Energy Geotechnics SEG-2018, Lausanne, Switzerland, 25-28 September 2018 (oral)

L. Paci, I. Rocchi, I.L. Fabricius, “Geotechnical challenges for a High Temperature Energy Storage in the greater Copenhagen area (Zealand, Denmark)”, International Symposium on Energy Geotechnics SEG-2018, Lausanne, Switzerland, 25-28 September 2018 (oral)

OCTOBER

Symposium in honor of the 25th work anniversary of Dr. Antoon ten Kate, 12 October 2018

Georgios M. Kontogeorgis, “Thermodynamics for a Sustainable Chemical Engineering in a Changing World - A pragmatic view”, Symposium in honor of the 25th work anniversary of Dr. Antoon ten Kate, Deventer, The Netherlands, 12 October 2018 (Invited talk)

Biophysical aspects of complexity in health and disease, 5th International Symposium, Milan, Italy, 12-13 October 2018

Nikolaj Sorgenfrei Blom, “DireWaves – Disarming Resistant Microbes with Resonant Waves”, Biophysical aspects of complexity in health and disease, 5th International Symposium, Milan, Italy, 12-13 October 2018 (Invited speaker)

SEG 88th annual meeting, Anaheim, CA, USA, 14-19 October 2018

T. Orlander, T. K.A. Andreassen, I.L. Fabricius, “Effective stress on deep sedimentary formations under non-isothermal conditions”, SEG 88th annual meeting, Anaheim, CA, USA, 14-19 October 2018 (oral)

3rd International Workshop on Thermal Methods for Enhanced Oil Recovery, Chendu, China 15-19 October 2018

E.H. Stenby, “compositional modeling for thermal EOR”, 3rd International Workshop on Thermal Methods for Enhanced Oil Recovery, Chendu, China 15-19 October 2018 (Invited Plenary Lecture)

D. Sandoval, E.H. Stenby, W. Yan, “Gas injection modeling in shale”, 3rd International Workshop on Thermal Methods for Enhanced Oil Recovery, Chendu, China 15-19 October 2018 (Oral)

13th Annual Conference on the Physics, Chemistry and Biology of Water, Sofia, Bulgaria, 18-21 October 2018

M. Bache, “Could a device used for CaCO₃ de-scaling change the properties of water itself?”, 13th Annual Conference on the Physics, Chemistry and Biology of Water, Sofia, Bulgaria, 18-21 October 2018 (Poster & poster award winner)

14th International Conference on Greenhouse Gas Control Technologies (GHGT-14), Melbourne, Australia, 21-25 October 2018

R. Neerup, J. K. Jørsboe, S. Almeida, S. H. B. Vinjarapu, A. Gladis, N. von Solms, K. Thomsen, P. L. Fosbøl, “Reaction kinetics of new innovative promoted CO₂ capture solvents”, 14th International Conference on Greenhouse Gas Control Technologies (GHGT-14), Melbourne, Australia, 21-25 October 2018 (Poster)

S. Almeida, D. Kloth, R. Neerup, A. Gladis, N. von Solms, P. L. Fosbøl, “Impact of Energy-Promoters/Additives on CO₂ capture, for biogas upgrading”, 14th International Conference on Greenhouse Gas Control Technologies (GHGT-14), Melbourne, Australia, 21-25 October 2018 (Poster)

P. L. Fosbøl, R. Neerup, S. Almeida, A. Rezazadeh, J. Gaspar, A. B. N. Knarvik, N. E. Flø, “Results of the third Technology Centre Mongstad campaign: FEED, process intensification, and simulation”, 14th International Conference on Greenhouse Gas Control Technologies (GHGT-14), Melbourne, Australia, 21-25 October 2018 (Poster)

R. Neerup, S. Almeida, K. Thomsen, R. Find, N. Z. R. Larsen, J. F. Poulsen, P. G. Kristensen, P. L. Fosbøl, “BioCO₂, a new Danish funded project for improved low cost biogas upgrading and pure CO₂ production”, 14th International Conference on Greenhouse Gas Control Technologies (GHGT-14), Melbourne, Australia, 21-25 October 2018 (Poster)

Liang Mu, Nicolas von Solms, “CO₂ storage by hydrate swapping – flooding experiments, thermal dissociation behavior and dissociation enthalpies,” 14th International Conference on Greenhouse Gas Control Technologies (GHGT-14), Melbourne, Australia, 21-25 October 2018 (Poster)

XI Iberoamerican Confence on Phase Equilibria and Fluid Properties for Process Design, Cordoba, Argentina, 21-25 October 2018

Georgios M. Kontogeorgis, “Advanced Equations of State – But how much have we advanced Science and Engineering?”, XI Iberoamerican Confence on Phase Equilibria and Fluid Properties for Process Design, Cordoba, Argentina, 21-25 October 2018 (Invited Plenary Lecture)

Georgios M. Kontogeorgis, “Industry-Academia Interactions: How to develop or improve them?” XI Iberoamerican Confence on Phase Equilibria and Fluid Properties for Process Design Cordoba (Argentina) 21-25 October 2018 (Round Table Discussion Presentation - Invited)

Commercial UAV EXPO Americas 2018, Las Vegas, USA, 28-30 October 2018

Mick Emil Kolster, Arne Døssing, Eduardo Lima Simões da Silva, “Magnetic surveying with UAVs”, Commercial UAV EXPO Americas 2018, Las Vegas, USA, 28-30 October 2018

Wind Energy Denmark, Hedensted, Denmark, 30-31 October 2018

A.P. Engsig-Karup, “Advances and challenges in hydrodynamic simulation methods”, Wind Energy Denmark, Hedensted, Denmark, 30-31 October 2018 (Invited speaker)

2018 AIChE Annual Meeting, Pittsburgh, PA, USA, 28 October-2 November 2018

E.L. Camacho Vergara, G.M. Kontogeorgis, X. Liang, “Modelling of Interfacial Tension and Adsorption of Inhomogeneous Systems with Classical Density Functional Theory”, 2018 AIChE Annual Meeting, Pittsburgh, PA, USA, 28 October-2 November 2018 (oral presentation)

NOVEMBER

Abu Dhabi International Petroleum Exhibition and Conference (ADIPEC) 2018, Abu Dhabi, United Arab Emirates, 12-15 November 2018

F.J. Kruger, G.M. Kontogeorgis, N. von Solms, “Application of uncertainty analysis in the design of subsea dehydration units”, Abu Dhabi International Petroleum Exhibition and Conference (ADIPEC) 2018, Abu Dhabi, United Arab Emirates, 12-15 November 2018 (poster)

DHRTC Technology Conference 2018, Copenhagen, Denmark, 12-13 November 2018

Hadise Baghooee, François Montel, Charlotte Lassen, Wei Yan, Alexander Shapiro, “Quality controlled PVT data from Lower Cretaceous chalk fields”, DHRTC Technology Conference 2018, Copenhagen, Denmark, 12-13 November 2018 (poster)

Ida A. Kirknel, Anders T. Schlaikjer, Kaj Thomsen, Philip L. Fosbøl, “Prediction of downhole scaling by thermodynamic calculations and production data”, DHRTC Technology Conference 2018, Copenhagen, Denmark, 12-13 November 2018 (poster)

Tian Wang, Simon Ivar Andersen, Alexander Shapiro, “Microfluidic control of oil droplet movement in capillaries”, DHRTC Technology Conference 2018, Copenhagen, Denmark, 12-13 November 2018 (poster)

Teresa Regueira, Erling H. Stenby, Wei Yan, “Experimental determination of phase behavior in tight Lower Cretaceous formation”, DHRTC Technology Conference 2018, Copenhagen, Denmark, 12-13 November 2018 (poster)

Ivanka Orozova-Bekkevold. “2D forward modelling of the overburden in the Valdemar field”, DHRTC Technology Conference 2018, Copenhagen, Denmark, 12-13 November 2018 (poster)

D.R. Sandoval, W. Yan, E.H. Stenby, “Modeling and Simulation of Oil Production from the Lower Cretaceous Tight Formation including Capillary Pressure Effects on Phase Behaviour”, DHRTC Technology Conference 2018, Copenhagen, Denmark, 12-13 November 2018 (poster)

C. Tsanas, E. H. Stenby, W. Yan, “Efficient calculation of multiphase geochemical reaction equilibrium for EOR applications”, DHRTC Technology Conference 2018, Copenhagen, Denmark, 12-13 November 2018 (poster)

Master Students 2018

D. C. Figueroa-Murcia, P. L. Fosbøl, K. Thomsen, “Modelling and experimental studies of scale formation at well conditions”, DHRTC Technology Conference 2018, Copenhagen, Denmark, 12-13 November 2018 (Oral)

C.S. Hemmingsen, A.P. Engsig-Karup, M. Byrne, K.K. Nielsen, “Coupled Systems for accurate well performance in reservoir simulators”, DHRTC Technology Conference 2018, Copenhagen, Denmark, 12-13 November 2018 (poster)

Wael F. Al-Masri, Alexander Shapiro, Wei Yan, “Gas liberation in Tight Porous Medium”, DHRTC Technology Conference 2018, Copenhagen, Denmark, 12-13 November 2018 (poster)

Jyoti S Pandey, Alexander Shapiro, Nicolas von Solms, “Kinetics of CH₄-CO₂ exchange in different mass transfer scenarios”, DHRTC Technology Conference 2018, Copenhagen, Denmark, 12-13 November 2018 (poster)

Yiqun Liu, Teresa Regueira, Erling H. Stenby, Wei Yan, “PVT study of gas-stock tank oil systems at HPHT conditions”, DHRTC Technology Conference 2018, Copenhagen, Denmark, 12-13 November, 2018 (poster)

DECEMBER

The Governmental Green Growth Team at DareDisrupt, Copenhagen, 4 December 2018

Nikolaj Sorgenfrei Blom, “Kan vand blive det nye vind?”/ “Could water become the new Wind?”, The Governmental Green Growth Team at DareDisrupt Skype-presentation from Japan to a group of top Danish CEOs, 4 December 2018 (invited speaker)

Exploring Water Molecular Systems in Nature, 3rd International Aquaphotomics Symposium, Awaji Island, Japan, 2-6 December 2018

Nikolaj Sorgenfrei Blom, “DireWaves – Disarming Resistant Microbes with Resonant Waves”, Exploring Water Molecular Systems in Nature, 3rd International Aquaphotomics Symposium, Awaji Island, Japan, 2-6 December 2018 (invited speaker)

Simon Brøndum Andersen
“How can Denmark and the Nordic countries become negative CO₂ emitters by 2040”
(Philip L. Fosbøl)

Hang Bian
“Investigation of Reservoir Parameters Related to Nanocellulose Injection in Oil Reservoir”
(Wei Yan)

Tessa Lund Biel-Nielsen
“Mass transfer from nano bubbles for anti-bacterial applications”
(Philip L. Fosbøl)

Maria Bonto
“Thermodynamic Analysis of Chalk-brine-oil Interactions”
(Alexander Shapiro)

Mohammadreza Mahdizadeh Dastjerdi
“Numerical modelling of DME-enhanced water injection in Heterogeneous Chalk Reservoirs”
(Alexander Shapiro)

Aditya Deepak Dixit
“Determination of Relative Permeabilities from Steady-State and Transient Experimental Data”
(Alexander Shapiro)

Wentao Gong
“Programming and thermodynamic modeling of aqueous salt system”
(Kaj Thomsen)

Mark Lusty Grandahl
“Geothermal Heat Production in Low Permeable Fractured Reservoirs”
(Alexander Shapiro)

Eirik Daviknes Hagerup
“Hydraulic fracturing in layered media”
(Alexander Shapiro)

Tablo Maref Hassan
“Development of low-temperature solid oxide electrolyses cells”
(Kaj Thomsen)

Ida Arent Kirknel
“Calculations and experiments concerning scaling/corrosion”
(Kaj Thomsen)

Mick Emil Kolster
“Exploring the impact of heat-flux anomalies derived from magnetic data on solid earth and cryosphere dynamics”
(Arne Døssing)

Wojciech Laskowski
“Designing Efficient p-Multigrid Strategies for the Laplace Equation – with application to a Spectral Element Fully Nonlinear Potential Flow Model”
(Allan Peter Ensig-Karup)

Frederik Winkel Lehn
“Well Spacing Optimization under Subsurface Uncertainty for Tight Carbonate Reservoirs”
(Nicolas von Solms)

Martin Due Olesen
“Thermodynamic modeling of the solubility of pharmaceuticals with the PC-SAFT EOS”
(Xiaodong Liang)

Andreas Ingeman Pedersen
“Modelling gas permeation in polymers used in liners for offshore applications”
(Nicolas von Solms)

Anna Samnioti
“Field Scale Long Term Optimization of a Gas Lift System”
(Wei Yan)

Michael Gram Sieverts
“Experimental Investigation of CH₄-CO₂ swapping in gas hydrates”
(Nicolas von Solms)

Yuntian Teng
“Experimental Study of Adding Nanocellulose into the Injection Water for Possible Enhancement of the Oil Recovery”
(Wei Yan)

Felix Terens
“Modelling Hydrate Formation for Hydrate Mitigation During Oil and Gas Production”
(Nicolas von Solms)

Athanasios Antonios Varsos
“Thermodynamics of petroleum fluids relevant to subsea processing”
(Nicolas von Solms)

Tianqing Wang
“CFD Simulation of Near Wellbore Flow Using Black Oil Description”
(Wei Yan)

Mark David Wigh
“Modeling of unexploded ordnance (UXO) by probabilistic inversion of synthetic and real magnetic data”
(Arne Døssing)

Aikaterini Zeneli
“Petrophysical interpretation of the Lark Formation”
(Ida Lykke Fabricius)

Tadeusz Sobczynski
“Petrophysics of organic rich chalk from Israel”
(Ida Lykke Fabricius)

Ismail Tayeb Muhammed El Hadi
“Effect of depletion and temperature on borehole stability
(Ivanka Orozova-Bekkevold and Tobias Orlander)

Publications

Published in 2018

CERE 1718 *“A three-dimensional model of two-phase flows in a porous medium accounting for motion of the separating surface”*

Alexander A. Shapiro
(Transport in Porous Media, 122 (2018) 1-32)

CERE 1719 *“New association schemes for mono-ethylene glycol: Cubic-Plus-Association parameterization and uncertainty analysis”*

Francois Kruger, Georgios Kontogeorgis, and Nicolas von Solms
(Fluid Phase Equilibria, 458 (2018) 211-233)

CERE 1720 *“Measurement of iron and lead sulfide solubility below 100°C”*

Diana Carolina Figueroa Murcia, Petter Lomsøy, Philip L. Fosbøl, Erling H. Stenby, and Kaj Thomsen
(Fluid Phase Equilibria, 475 (2018) 118-126)

CERE 1721 *“Application of a crossover equation of state to describe phase equilibrium and critical properties of n-Alkanes and Methane/n-alkane mixtures”*

Andre P.C.M. Vinhal, Wei Yan, and Georgios M. Kontogeorgis
(J. Chem. Eng. Data, 63 (4) (2018) 981-993)

CERE 1723 *“The Debye-Hückel theory and its importance in modeling electrolyte solutions”*

Georgios M. Kontogeorgis, Bjørn Maribo-Mogensen, and Kaj Thomsen
(Fluid Phase Equilibria, 462 (2018) 130-152)

CERE 1725 *“An algorithm for gradient-based dynamic optimization of UV flash processes”*

Tobias K.S. Ritschel, Andrea Capolei, Jozsef Gaspar, and John Bagterp Jørgensen
(Computers and Chemical Engineering, 114 (2018) 281-295)

CERE 1727 *“Thermodynamic modeling of relevance to natural gas processing”*

Georgios M. Kontogeorgis, and Eirini Karakatsani (Chapter in the book “Natural Gas Processing from Midstream to Downstream”, Edited by Namir Elbashir, Mahmoud El-Halwagi, Ioannis Economou, and Ken Hall)

CERE 1628 *“Near-wellbore modeling of a horizontal well with Computational Fluid Dynamics”*

Márton L. Szanyi, Casper S. Hemmingsen, Wei Yan, Jens H. Walther, and Stefan L. Glimberg
(Journal of Petroleum Science and Engineering, 160 (2018) 119-128)

CERE 1729 *“Antifreeze proteins and gas hydrate inhibition”*

Nicolas von Solms
(Chapter in the book “Antifreeze proteins, Volume II – Biochemistry, Molecular Biology, Physical-chemistry and Applications, Edited by Hans Ramløv and Dennis Friis, Springer Verlag)

CERE 1730 *“Hydrate thermal dissociation behavior and dissociation enthalpies in methane-carbon dioxide swapping process”*

Liang Mu, and Nicolas von Solms
(J. Chem. Thermodynamics 117 (2018) 33-42)

CERE 1731 *“CO₂ mass transfer model for carbonic anhydrase-enhanced aqueous MDEA solutions”*

Arne Gladis, Maria T. Gundersen, Randi Neerup, Philip L. Fosbøl, John M. Woodley, and Nicolas von Solms
(Chemical Engineering Journal, 335 (2018)197-208)

CERE 1744 *“Low field NMR surface relaxivity studies of chalk and argillaceous sandstones”*

Konstantina Katika, Henrik Fordsmand, and Ida L. Fabricius
(Microporous and Mesoporous Materials, 269 (2018) 122-124)

CERE 1801A *“Numerical aspects of phase equilibrium calculations with the cubic and association models”*

Xiaodong Liang
(Ind. Eng. Chem. Res., 57 (2018) 14273-14285)

CERE 1802 *“Elasticity and electrical resistivity of chalk and greensand during water flooding with selective ions”*

K. Katika, M.M. Alam, A. Alexeev, K.H. Chakravarty, P.L. Fosbøl, A. Revil, E. Stenby, I. Xiarchos, A. Yousefi, and I.L. Fabricius
(Journal of Petroleum Science and Engineering, 161 (2018) 204-218)

CERE 1803 *“Extensive study of the capabilities and limitations of the CPA and sPC-SAFT equations of state in modeling a wide range of acetic acid properties”*

Rafael T.C.S. Ribeiro, André L. Alberton, Márcio L.L. Paredes, Georgios M. Kontogeorgis, and Xiaodong Liang
(Ind. Eng. Chem. Res., 57 (2018) 5690-5704)

CERE 1804 *“Recent advances with association models for practical applications”*

Ioannis Tsivintzelis, Martin Gamel Bjørner, and Georgios M. Kontogeorgis
(Molecular Physics, 116 (2018) 1921-1944)

CERE 1805 *“Draft: Nonlinear wave-body interaction using a mixed-eulerian-lagrangian spectral element model”*

Carlos Monteserin Sanchez, Allan P. Ensig-Karup, and Claes Eskilsson (Proceedings of the 37th International Conference on Ocean, Offshore and Arctic Engineering, OMAE 2018, June 17-22, 2018, Madrid, Spain)

CERE 1807 *“Influence of adsorption and capillary pressure on phase equilibria inside shale reservoirs”*

Diego R. Sandoval, Wei Yan, Michael L. Michelsen, and Erling H. Stenby
(Energy & Fuels, 32 (2018) 2819-2833)

CERE 1808 *“Extension of modified RAND to multiphase flash specifications based on state functions other than (T,P)”*

Duncan Paterson, Michael L. Michelsen, Wei Yan, Erling H. Stenby
(Fluid Phase Equilibria, 458 (2018) 288-299)

CERE 1809 *“RAND-based formulations for isothermal multiphase flash”*

Duncan Paterson, Michael L. Michelsen, Erling H. Stenby, and Wei Yan
(SPE 182706 (2018))



<p>CERE 1810 <i>“Improvement of the PR-CPA equation of state for modelling of acid gases solubilities in aqueous alkanolamine solutions”</i></p> <p>Tianyuan Wang, Elise El Ahmar, Christophe Coquelet, and Georgios M. Kontogeorgis (Fluid Phase Equilibria, 471 (2018) 74-87)</p>	<p>CERE 1815 <i>“Experimental study of the aqueous CO₂-NH₃ rate of reaction for temperatures from 15° C to 35° C, NH₃ concentrations from 5% to 15% and CO₂ loadings from 0.2 to 0.6.”</i></p> <p>Stafano Lillia, Davide Bonalumi, Philip L. Fosbøl, Kaj Thomsen, and Gianluca Valenti (International Journal of Greenhouse Gas Control, 70 (2018) 117-127))</p>	<p>CERE 1826 <i>“Computation of Phase Equilibrium in Reservoir Simulation and Optimization”</i></p> <p>Tobias K.S. Ritschel and John Bagterp Jørgensen (IFAC PapersOnLine, 51-8 (2018) 94-101) (Proceedings of the 3rd IFAC Workshop on Automatic Control in Offshore Oil and Gas Production, May 30 – June 1, 2018, Esbjerg, Denmark)</p>	<p>CERE 1834 <i>Efficient ionic liquid-based platform for multi-enzymatic conversion of carbon dioxide to methanol”</i></p> <p>Zhibo Zhang, Jan Muschiol, Yuhong Huang, Sigyn Björk Sigurdardóttir, Nicolas von Solms, Anders E. Daugaard, Jiang Wei, Jianquan Luo, Bao-Hua Xu, Suojing Zhang, and Manuel Pinelo (Green Chemistry, 20 (2018) 4339-4348)</p>
<p>CERE 1811 <i>“Ternary vapor-liquid equilibrium measurements and modeling of ethylene glycol (1) + water (2) + methane (3) systems at 6 and 12.5 MPa”</i></p> <p>Francois J. Kruger, Marie V. Danielsen, Georgios M. Kontogeorgis, Even Solbraa, and Nicolas von Solms (J. Chem. Eng. Data, 63 (2018) 1789-1796)</p>	<p>CERE 1816 <i>“Low energy recycling of ionic liquids via freeze crystallization during cellulose spinning”</i></p> <p>Yanrong Liu, Anne S. Meyer, Yi Nie, Suojiang Zhang, and Kaj Thomsen (Green Chemistry, 20 (2018) 493-501)</p>	<p>CERE 1827 <i>“Nonlinear Filters for State Estimation of UV Flash Processes”</i></p> <p>Tobias K.S. Ritschel and John Bagterp Jørgensen (Proceedings of the 2nd IEEE Conference on Control Technology and Applications, August 21-24, 2018, Copenhagen, Denmark)</p>	<p>CERE 1835 <i>“Characterization of emulsion formation with nanoparticles for enhanced oil recovery”</i></p> <p>Muhammad Waseem Arshad, Karen Louise Feilberg, Alexander Shapiro, and Kaj Thomsen (SPE-192170-MS (2018))</p>
<p>CERE 1812 <i>“Spectral/hp element methods: Recent developments, applications, and perspectives”</i></p> <p>Hui Xu, Chris D. Cantwell, Carlos Monteserin, Claes Eskilsson, Allan P. Ensig-Karup, and Spencer J. Sherwin (Journal of Hydrodynamics, 30 (2018) 1-22)</p>	<p>CERE 1820 <i>“An Open-source Thermodynamic Software Library”</i></p> <p>Tobias K.S. Ritschel, Jozsef Gaspar, Andrea Capolei, and John Bagterp Jørgensen (DTU Compute Technical Report-2016-12, Department of Applied Mathematics and Computer Science, Technical University of Denmark)</p>	<p>CERE 1830 <i>“Multicomponent vapor-liquid equilibrium measurement and modeling of ethylene glycol, water and natural gas mixtures at 6 and 12.5 MPa”</i></p> <p>Francois J. Kruger, Georgios M. Kontogeorgis, Even Solbraa, and Nicolas von Solms (J. Chem. Eng. Data, 63 (2018) 3628-3639)</p>	<p>CERE 1836 <i>“Modeling hydrofluoroolefins with the CPA and PC-SAFT Equations of State”</i></p> <p>Kai Kang, Xiaopo Wang, Georgios M. Kontogeorgis, and Xiaodong Liang (Ind. Eng. Chem. Res., (2018) 17289-17300)</p>
<p>CERE 1813 <i>“A novel equipment-friendly and environment-friendly well stimulation fluid for carbonate reservoirs: Better wormholes and lower corrosion at reservoir conditions</i></p> <p>J. S. Pandey, N. Nazari, K. Thomsen, and R. Barati (SPE 189496-MS (2018))</p>	<p>CERE 1821 <i>“Computation of Phase Equilibrium and Phase Envelopes”</i></p> <p>Tobias K.S. Ritschel and John Bagterp Jørgensen (DTU Compute Technical Report-2017-11, Department of Applied Mathematics and Computer Science, Technical University of Denmark)</p>	<p>CERE 1832 <i>“Experimental study on methane production from hydrate-bearing sandstone by flue gas swapping”</i></p> <p>Liang Mu, and Nicolas von Solms (Energy Fuels, 32 (2018) 8167-8174)</p>	<p>CERE 1837 <i>“Developing coarse-grained model for 1-alkyl-3-methyl-imidazolium chloride ionic liquids”</i></p> <p>Jiahuan Tong, Yandong Guo, Feng Huo, Xiaodong Xie, Hong-Yan He, Nicolas von Solms, Xiaodong Liang, and Suojiang Zhang (Industrial & Engineering Chemistry Research, 57 (2018) 15206-15215)</p>
<p>CERE 1814 <i>“Experimental data of the aqueous NH₃ and CO₂ absorption at temperatures from 15 C to 35 C, NH₃ concentrations from 5% to 15% and CO₂ loadings from 0.2 to 0.6 measured with the Wetted Wall Column”</i></p> <p>Stafano Lillia, Davide Bonalumi, Philip L. Fosbøl, Kaj Thomsen, and Gianluca Valenti (Data in Brief, 17 (2018) 1240-1244)</p>	<p>CERE 1825 <i>“The Extended Kalman Filter for State Estimation of Dynamic UV Flash Processes”</i></p> <p>Tobias K.S. Ritschel and John Bagterp Jørgensen (IFAC PapersOnLine, 51-8 (2018) 164-169) (Proceedings of the 3rd IFAC Workshop on Automatic Control in Offshore Oil and Gas Production, May 30 - June 1, 2018, Esbjerg, Denmark)</p>	<p>CERE 1833 <i>“Ionic liquids as bifunctional cosolvents enhanced CO₂ conversion catalyzed by NADH-dependent formate dehydrogenase”</i></p> <p>Zhibo Zhang, Bao-hua Xu, Jianquan Luo, Nicolas von Solms, Hongyan He, Yaqin Zhang, Manuel Pinelo, and Suojiang Zhang (Catalysts, 8 (2018) 304-)</p>	<p>CERE 1839 <i>“Solubility of syngas components in water acetic acid and alcohol using new standard fugacity methodology”</i></p> <p>Mauro Torli, Luydmila Geer, Georgios Kontogeorgis, and Philip Fosbøl (Ind. Eng. Chem. Res., 57 (2018) 16958-16977)</p>



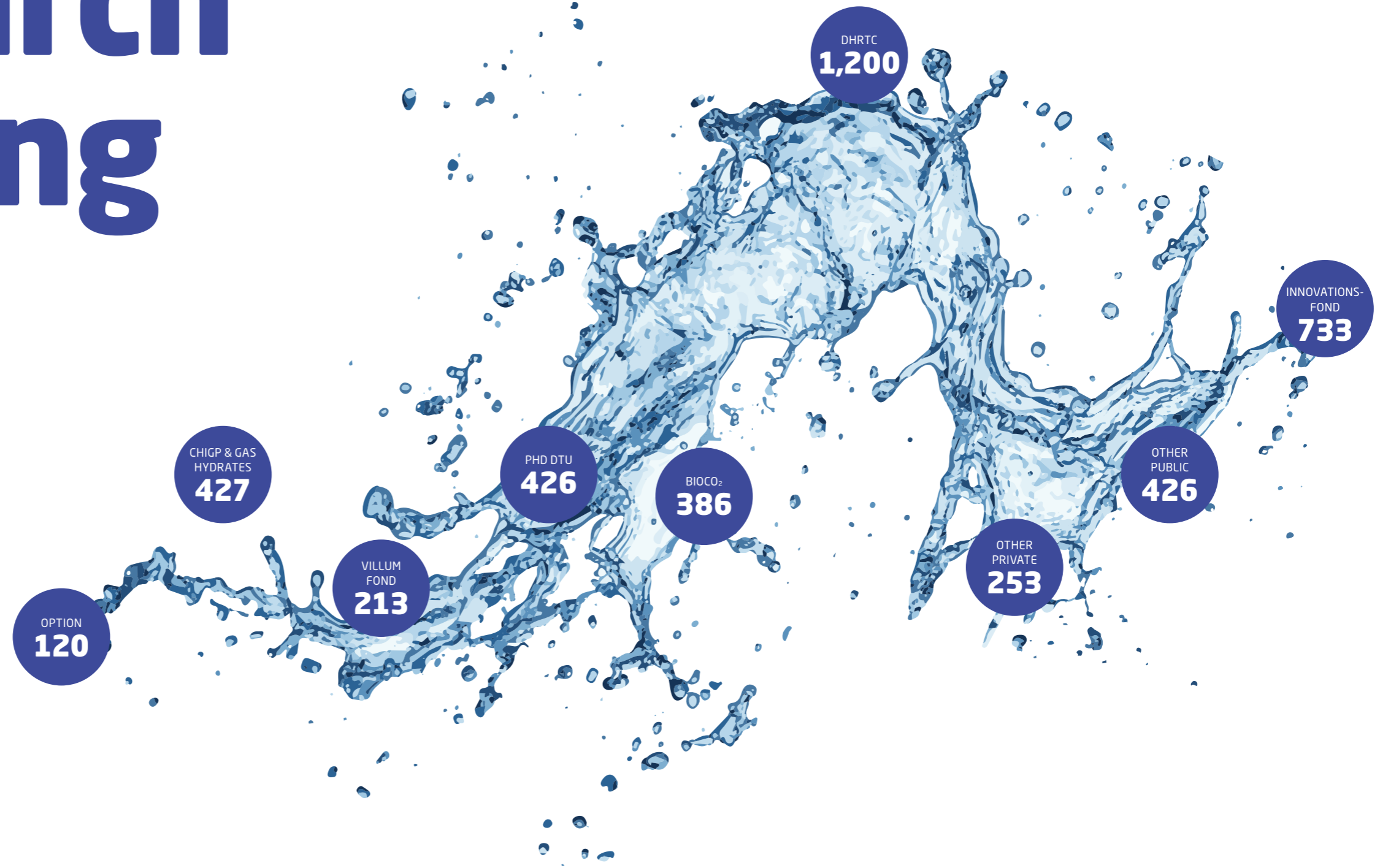
<p>CERE 1840 “Application of uncertainty analysis in the design of subsea natural gas dehydration units”</p> <p>Francois J. Kruger, Georgios M. Kontogeorgis, and Nicolas von Solms (SPE-192822-MS (2018))</p>	<p>CERE 1848 “Thermal conductivity of sandstones from Biot’s coefficient”</p> <p>A.A. Marczyński, E. Adamopoulou, H. Milsch, I.L. Fabricius, J.J. Asmussen, L. Pasquinelli and T. Orlander (Geophysics 83 (2018) D173-D185)</p>	<p>CERE 1859 “Combined polyhydroxyalkanoates (PHA) and 1, 3-propanediol production from crude glycerol: Selective conversion of volatile fatty acids into PHA by mixed microbial consortia”</p> <p>Anna Burniol-Figols, Cristiano Varrone, Simone B. Lee, Ioannis V. Skiadas, Hariklia N. Gavala (Water Research, 136 (2018), 180-191)</p>	<p>CERE 1867 “A spectral/hp element depth-integrated model for nonlinear wave-body interaction”</p> <p>Umberto Bosi, Allan P. Ensig-Karup, Claes Eskilsson, and Mario Ricchiuto (Available online at www.sciencedirect.com. Comput. Methods Appl. Mech. Engrg. (2018) 1-15)</p>
<p>CERE 1844 “Syngas biomethanation: State-of-the-art review and perspectives”</p> <p>Antonio Grimalt-Aleman, Ioannis V. Skiadas and Hariklia N. Gavala (Biofuels, Bioprod Biorefining, 12 (2018) 139–158)</p>	<p>CERE 1849 “Incorporating electrostatic effects into the effective stress relation – insights from chalk experiments”</p> <p>A. Nerموen, E. Storm, I.L. Fabricius, M.V. Madland, R.I. Korsnes and T. Stodle (Geophysics 83 (2018) 123-135)</p>	<p>CERE 1860 “Polyhydroxyalkanoates (PHA) production from fermented crude glycerol: Study on the conversion of 1, 3-propanediol to PHA in mixed microbial consortia”</p> <p>Anna Burniol-Figols, Cristiano Varrone, Simone B. Lee, Ioannis V. Skiadas, Hariklia N. Gavala (Water Research, 128 (2018), 255-266)</p>	<p>CERE 1869 “Screening wells by multi-scale grids for multi-stage Markov Chain Monte Carlo simulation”</p> <p>Hani Akbari, and Allan P. Ensig-Karup (Mathematics and Computers in Simulation, 151 (2018) 15-28)</p>
<p>CERE 1845 “Enrichment of syngas-converting mixed microbial consortia for ethanol production and thermodynamics-based design of enrichment strategies”</p> <p>Antonio Grimalt-Aleman, Mateusz Łężyk, Lene Lange, Ioannis V. Skiadas and Hariklia N. Gavala (Biotechnol Biofuels, 11 (2018) 1–22)</p>	<p>CERE 1850 “Temperature cycling and its effect on stress-strain relationships in high porosity chalks”</p> <p>A. Nerموen, I.L. Fabricius, R.I. Korsnes and T. Voake. (Journal of Rock Mechanics and Geotechnical Engineering (2018))</p>	<p>CERE 1863 “Study of the Feasibility of the Carbon Dioxide Injection in a North Sea Petroleum Reservoir”</p> <p>Wael Al-Masri, Christos Pappaspyrou, and Alexander Shapiro (SPE-190783-MS) (Presented at the SPE Europec featured at 80th EAGE Conference and Exhibition, Copenhagen, Denmark, 11-14 June, 2018)</p>	<p>CERE 1873 “Nonlinear Wave-Body Interaction Using a Mixed-Eulerian-Lagrangian Spectral Element Model”</p> <p>Carlos Monteserin Sanchez, Allan P. Ensig-Karup, and Claes Eskilsson (Proceedings of the 37th International Conference on Ocean, Offshore and Arctic Engineering, OMAE 2018, Madrid, Spain, 17-22 June, 2018)</p>
<p>CERE 1846 “Interpretational challenges related to studies of the chalk particle surface in scanning and transmission electron microscope”</p> <p>I.L. Fabricius, M.L. Hjuler and V.F. Hansen (Bull. Geol. Soc. Denmark. 66 (2018) 151-165)</p>	<p>CERE 1854 “Failure characterization in geomechanical testing using Nuclear Magnetic Resonance spectroscopy”</p> <p>C. Ravnås, I.L. Fabricius, L.T.P. Meireles and M.J. Welch (in Lawrence, Preene, Lawrence and Buckley (eds), Engineering in Chalk September 17-18 2018, London. 541-547. ISBN 978-0-7277-6407-2 https://doi.org/10.1680/eiccf.64072.541 ICE Publishing)</p>	<p>CERE 1865 “Spectral Element FNPF Simulation of Focused Wave Groups Impacting a Fixed FPSO”</p> <p>Allan P. Ensig-Karup, and Claes Eskilsson (Proceedings of the 28th International Ocean and Polar Engineering Conference, Sapporo, Japan, 10-15 June 2018, pp. 1443-1450)</p>	<p>CERE 1874 “A High-Order Spectral Element Unified Boussinesq Model for Floating Point Absorbers”</p> <p>Umberto Bosi, Allan P. Ensig-Karup, Claes Eskilsson, Mario Ricchiuto, and Elie Solat (Proceeding of the 36th International Conference for Coastal Engineering, ICCE 2018, Baltimore, Maryland, USA, 30 July - 3 August)</p>
<p>CERE 1847 “Elasticity and electrical resistivity of chalk and greensand during water flooding with selective ions”</p> <p>A. Alexeev, A. Revil, A. Yousefi, E. Stenby, I.L. Fabricius, I. Xiarchos, K.H. Chakravarty, K. Katika, M.M. Alam and P.L. Fosbøl (Journal of Petroleum Science and Engineering 161 (2018) 204-218)</p>	<p>CERE 1855 “Investigation of controlling parameters on geomechanical properties of the Southern Danish Central Graben chalk”</p> <p>E.M. Storebø, I.L. Fabricius, L.P. Meireles and M.J. Welch (in Lawrence, Preene, Lawrence and Buckley (eds), Engineering in Chalk September 17-18 2018, London. 681-686. ISBN 978-0-7277-6407-2 https://doi.org/10.1680/eiccf.64072.541 ICE Publishing)</p>	<p>CERE 1866 “Numerical Simulations of Peregrine Breathers Using a Spectral Element Model”</p> <p>Dimitrios Koukounas, Claes Eskilsson, and Allan P. Ensig-Karup (Proceedings of the 37th International Conference on Ocean, Offshore and Arctic Engineering, OMAE, 2018, Madrid, Spain, 17-22 June, 2018)</p>	<p>CERE 1877 “An offshore reservoir monitoring system based on fiber optic sensing of seabed strains”</p> <p>E. Levenberg, I. Orozova-Bekkevold, K. Nielsen (DHRTC Report “Radical Innovation-Results of the Radical Innovation Sprint 2017”, p. 13-23. Published on the DHRTC website August 9th, 2018)</p>

Publications

Submitted in 2018

<p>CERE 1801 <i>“On the isobaric-isothermal flash calculations”</i></p> <p>Xiaodong Liang (Internal report)</p>	<p>CERE 1838 <i>“Modeling the phase behavior of bitumen/n-alkane systems with the cubic plus association (CPA) equation of state”</i></p> <p>Yechun Zhang, Alay Arya, Georgios Kontogeorgis, and Harvey Yarranton (Submitted for publication)</p>	<p>CERE 1861 <i>“Biocarbonate Flooding of Homogeneous and Heterogeneous Cores from a Carbonaceous Petroleum reservoir”</i></p> <p>Samira Mohammadkhani, Alexander Shapiro, Hamidreza Shahverdi, Sidsel Marie Nielsen, and Mohsen Nasr Esfahny (Submitted for publication)</p>	<p>CERE 1872 <i>“A Blind Comparative Study of Focused Wave Interactions with a Fixed FPSO-like Structure (CCP-WSI Blind Test Series 1)”</i></p> <p>N.E. Ransley, S. Yan, S. Brown, T. Mai, D. Graham, D. Greaves, Q. Ma, P.H. Musiedlak, A. P. Engsig-Karup, C. Eskilsson, Qian Li, J. Wang, Z. Xie, V. Sriram, T. Stoesser, Y. Zhuang, Qi Li, D. Wan, G. Chen, H. Chen, L. Qian, Z. Ma, D. Causon, C. Mingham, I. Gatin, H. Jasak, V. Vukcevic, S. Downie, P. Higuera, E. Buldakov, D. Stagonas, Q. Cheng, J. Zang (Submitted for publication)</p>
<p>CERE 1806 <i>“Multiphase coupling of a reservoir simulator and computational fluid dynamics for accurate near-well flow”</i></p> <p>Casper Schytte Hemmingsen, Stefan Lemvig Glimberg, Nathan Quadrio, Carsten Volcker, Kenny Krogh Nielsen, Jens Honore Walther, Michael Byrne, and Allan Peter Engsig-Karup (Submitted for publication)</p>	<p>CERE 1842 <i>“Comparison of two crossover procedures for describing thermodynamic behavior from singular critical to regular classical regions”</i></p> <p>Asma Jamali, Andre P.C.M. Vinhal, Hassan Behnejad, Wei Yan, and Georgios M. Kontogeorgis (Submitted for publication)</p>	<p>CERE 1862 <i>“Mechanisms of smart waterflooding in carbonate oil reservoirs – a review”</i></p> <p>Jiasheng Hao, Samira Mohammadkhani, Hamidreza Shahverdi, Mohsen Nasr Esfahny, and Alexander Shapiro (Submitted for publication)</p>	
<p>CERE 1828 <i>“Nonlinear Model Predictive Control for Disturbance Rejection in Isoenergetic-isochoric Flash Processes”</i></p> <p>Tobias K.S. Ritschel and John Bagterp Jørgensen (Accepted by the 12th IFAC Symposium on Dynamics and Control of Process Systems, including Biosystems, April 23-26, 2019, Florianopolis, Brazil)</p>	<p>CERE 1843 <i>Corrigendum to “Improvement of the PR-CPA equation of state for modelling of acid gases solubilities in aqueous alkanolamine solutions”</i></p> <p>Tianyuan Wang, Philippe Guittard, Christophe Coquelet, Elise El Ahmar, Oliver Baudouin, and Georgios M. Kontogeorgis (Submitted for publication)</p>	<p>CERE 1864 <i>“A Stabilised Mixed Eulerian Lagrangian Spectral Element Method for Nonlinear Wave Interaction with Fixed Structures”</i></p> <p>Allan Peter Engsig-Karup, Carlos Monteserin, and Claes Eskildsson (Submitted for publication)</p>	
<p>CERE 1829 <i>“Production Optimization of Thermodynamically Rigorous Isothermal and Compositional Models”</i></p> <p>Tobias K.S. Ritschel and John Bagterp Jørgensen (Presented at the 16th European Conference on the Mathematics of Oil Recovery, September 3-6, 2018, Barcelona, Spain)</p>	<p>CERE 1857 <i>“Stiffening and strengthening by increased temperature of dry sandstones from the deep North Sea Basin”</i></p> <p>I.L. Fabricius, K.A. Andreassen and T. Orlander (80th EAGE Conference and Exhibition 11-14 June 2018, Copenhagen, Denmark, Extended abstract, 4p.)</p>	<p>CERE 1870 <i>“A Multiscale Direct Solver for the Approximation of Flows in High Contrast Porous Media”</i></p> <p>Hani Akbari, Victor Ginting, Allan Engsig-Karup, and Felipe Pereira (Submitted for publication)</p>	
<p>CERE 1831 <i>“Estimation of reserves and production potential of newly discovered naturally fractured reservoirs”</i></p> <p>Justin Brand Ferrell (Accepted by Croatian Oil & Gas Journal)</p>	<p>CERE 1858 <i>“Effective stress on deep sedimentary formations under non-isothermal conditions”</i></p> <p>I.L. Fabricius, K.A. Andreassen and T. Orlander (SEG 88th annual meeting, 14-19 October, 2018, Anaheim, CA, USA, Extended abstract DOI: 10.3997/2214-4609.201801607 , 3507-3511)</p>	<p>CERE 1871 <i>“Efficient Physics-Based Model Order Reduction for Large Scale Reservoir Simulation”</i></p> <p>Hani Akbari, and Allan Peter Engsig-Karup (Submitted for publication)</p>	

Research Funding



Research Funding 2018

As a university research center our objective is to spend all of our money on research. No management bonuses or other dividends are due, and gradually all funding received will be invested with the aim of maximizing the production of high-quality research results and highly skilled researchers at PhD and Postdoc level.

The research carried out in CERE is funded by grants from a number of public and private sponsors. The external funding received in 2018 fell under the following projects and categories (all amounts in kEUR):

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

Publications in 2018. The full list of 2018 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. The list of 2018 Master's Theses is found in the e-report.