DTU

Center for Energy Resources Engineering

CERE 2020 Annual Report

CERE Annual Report 2020
Publisher:
CERE, Center for Energy Resources Engineering
Technical University of Denmark (DTU) Building 229
DK-2800 Kgs. Lyngby, Denmark

Phone: +45 45 25 28 67
Fax: +45 45 88 22 58

Website:
www.cere.dtu.dk

Editor-in-chief:
Nicolas von Solms, Chairman of CERE

Assistant Editors:
Anne Louise Biede, Administrative Coordinator, CERE
Patricia Wagner, Project Administrator, CERE

Text:
Morten Andersen, science reporter
www.manjourn.dk

Layout:
Christian Ove Carlsson, CERE

Photos – unless otherwise stated:
Christian Ove Carlsson, CERE

Cover photo shows the oxidation of a rust product ($FeCO_3$). Understanding the behaviour of $FeCO_3$ is essential for limiting corrosion in processes where CO_2 is handled. Such processes could be CO_2 capture, transport, storage and utilisation, which are some of the needed tools to mitigate the anthropogenic greenhouse gasses.

Contents

A Research Center in Good Health

Hardly any research organization in the world has been entirely unaffected by the COVID-19 pandemic. At CERE, while we fortunately did not see staff or students becoming severely ill with the virus, we obviously felt the challenges associated with lockdowns beginning in March and lasting for the rest of 2020. Still, I am pleased to report that collectively we were able to continue our activities in both research and education at a close-to-normal pace. I am certain, that several of the digital tools and changed workflows that we were compelled to introduce will survive into the post-pandemic reality.

Before I go deeper into the various developments, I should probably explain the reason why you see a new name and portrait below this introduction. 2020 marked a changing of the guards in the leadership of CERE. In November, I succeeded Professor Georgios M. Kontogeorgis who had been head of the center since July 2014. There is little doubt that the center's success during the past seven years can to a large extent be attributed to the leadership and tireless efforts which Georgios devoted to the task.

Thus, it is with a sense of both honor and great responsibility that I take over this position following in the footsteps of Georgios and of Professor Erling H. Stenby, who was head of the center during its first 20 years. For the entire history of CERE, the industrial Consortium has been one of our greatest strengths. As chairman I will continue this tradition, consolidating and strengthening collaboration with our Consortium members.

Momentum for carbon capture

Another CERE characteristic is the cross-disciplinary academic profile, spanning across several departments at DTU – Chemical Engineering, Chemistry, Compute, Civil Engineering, and Space. This unique construction enables an interdisciplinary approach to solving large problems. An example here is Carbon Capture Utilization and Storage (CCUS). Not least thanks to the dedication of Associate Professor Philip L. Fosbøl, heading several projects, CERE has remained committed to CCUS, and is well suited to lead now as there is momentum in this area. I am confident we will be able to initiate larger projects involving several departments.

Fortunately, Georgios has not left us – as is evident from several of the articles in this annual report. Georgios is very visible in research and research leadership. Among his duties is coordination of a large European program on electrolyte system modelling. Members of our industrial Consortium have shown significant interest in this field, which continues to be a key area for CERE, also after the retirement of one of its pioneers, Associate Professor Kaj Thomsen.

Another traditional CERE stronghold, hydrocarbon research, will continue to play an important role. For some years now, several oil and gas projects have been carried out in close collaboration with DHRTC (Danish Hydrocarbon Research and Technology Center) at DTU. The CERE-DHRTC collaboration continues to produce high-quality research and education. I note with pride that a recent QS World University ranking assessed the petroleum engineering environment at DTU – with Associate Professor Alexander Shapiro as head of studies - to be one of the worlds' finest.

Flash, water, and biorefining

Flash calculations – algorithms for predicting the amount of evaporation taking place due to pressure drop when a liquid stream passes through a confinement for instance at a production plant – is another CERE classic. This field is closely related to the name of an iconic CERE faculty member, the late Michael L. Michelsen, whom we lost in 2020. He was a highly active Emeritus, and had scientific manuscripts pending when he passed away. His heritage lives on at CERE, with a major breakthrough seen in 2020: A team headed by Associate Professor Wei Yan has shown how one can extend the use of flash algorithms for environments outside industrial plants.

Further, we continue to be active in bioenergy and biorefining. Fermentation of syngas and similar biological processes have emerged as attractive, green methods for production of fuels and chemicals. The first industrial breakthroughs have come, and research into ways to increase yields and optimize economic feasibility for a range of products continues at high pace with Associate Professor Hariklia N. Gavala as leader.
A relatively new field for CERE 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 will continue exploring it, not least since breakthroughs here will have implications in some of the strategic areas for CERE. Senior Scientist Michael Bache heads an important new project here.

Hope to see you in person soon!

As I mentioned above, CERE was of course affected by the COVID-19 lockdowns in Denmark. What might be more surprising to our stakeholders is the fact that CERE is also involved in actual COVID-19 mitigation planning. CERE faculty members, Professor John Bagterp Jørgensen and Associate Professor Allan P. Engsig-Karup, take part in a project on development of computational decision-making tools for pandemic management.

I applaud their success in this area. I am proud of the way our dedicated faculty and researchers, assisted by our skilled technical and administrative personnel, and our students have handled this highly unusual year. It has been a true pleasure to see you all make the best of not least the available digital resources, including an almost completely virtual version of our Discussion meeting with industry Consortium member participation in June 2020, and the summer course on advanced thermodynamics in August 2020 in a digital format. Still, I miss seeing you all in person for these and other CERE events, and I hope that we can finally actually meet in the near future!

Professor Nicolas von Solms,
Chairman of CERE

Industry Consortium

The Consortium – our Strongest Asset

CERE is supported by public means obtained from several sources through competitive grants, e.g. Innovation Fund Denmark, EU framework programs for science and innovation, and The Danish Research Councils. The center is also supported by grants from several private companies.

However possibly the strongest asset of CERE is the industrial Consortium. Approximately 25 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.

CERE Consortium:

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- Exxon Mobil
- DSM
- Equinor
- HESS
- IFPEN
- KBC
- Linde
- MOL
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Carbon Capture

Mobile carbon capture unit at the public sewage treatment plant Mølleåværket

Takeoff for Carbon Capture

A stubborn dedication has positioned CERE as a frontrunner in the race to implement Carbon Capture and Storage at full scale.

"Once you ignite a rocket and it lifts off, everybody sees it. Including those who never took any notice during the years it took to design and build it."

According to Associate Professor Philip L. Fosbøl, heading the Carbon Capture and Storage (CCS) activities at CERE, the metaphor suits the current situation: CCS has really taken off.

"It is almost surreal. We have never seen a level of activity like this. We are planning several new pilot and demonstration facilities. A handful of industrial partners and end-users are already onboard, and several additional projects are in the making pending on discussions with potential partners."

The crown jewel of the CCS activities at CERE is a mobile carbon capture unit built by industrial partner Pentair (previously Union Engineering) in co-operation with CERE. The unit is currently in action at the public sewage treatment plant Mølleåværket not far from the DTU campus. The unit is able to remove one ton of CO_2 per day.

A breakthrough in economic feasibility

Just like at most other state-of-the-art pilot and demonstration facilities, the fundamental capture technology at the mobile unit is amine-based. The innovations lie elsewhere:

"What we have built is far from a standard carbon capture unit. It has every fancy supplementary feature we were able to think of. This is necessary, because our ambition is not just capturing large quantities of CO_2. We intend to optimize the quality of the captured CO_2 to make it useful as a raw material, and even more importantly, we aim to improve overall economic feasibility dramatically."

Through finetuning of the involved processes, CERE and its partners are on route to reduce the overall energy consumption by as much as 45 %.

"This will translate into cutting the costs of carbon capture almost in half, since energy consumption is by far the heaviest component in terms of costs. Needless to say, a cost reduction of this magnitude will dramatical-

ly improve the outlook for full-scale carbon capture implementation."

Survived a decline in funding

The means to achieve the dramatic reduction in energy consumption are found in classic chemical engineering disciplines such as process optimization, optimization of liquid composition, and the use of heat pumps to minimize energy losses.

"It is highly satisfying to see, how the advanced thermodynamics which have always been a core activity at CERE can be applied in a way that really changes the reality of a technology of huge societal importance," Philip L. Fosbøl reflects.

Looking at the history of CERE's carbon capture engagement, it has not always been obvious that this field would survive at the center. On several occasions, the activities have been starved in terms of funding, and the current success can largely be attributed to the stubbornness of the involved researchers and the CERE management.

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.

"As recently as in 2017, it was simply impossible to raise funding for CCS research from Danish sources," Philip L. Fosbøl recalls.

Partner in leading EU projects

Still, some public programs remained, mainly in EU and Norway. Active participation in these collaborations allowed CERE to maintain its level of research in the field.

For instance, CERE is a partner in the so-called 3D project funded mainly by the EU framework program Horizon 2020. The three Ds denote "DMX Demonstration in Dunkirk". At the Arcelor-Mittal steel factory in Dunkirk, France, a consortium led by IFP Energies Nouvelles (a member of the CERE industry Consortium) operates a demonstration plant able to capture 0.5 metric tons of CO_2 per hour. DMX is a carbon capture technology patented by IFP Energies Nouvelles. The contributions from CERE are coordinated by Associate Professor Philip L. Fosbøl and Professor Nicolas von Solms.

Also, CERE is a partner in another Horizon 2020 project named Consensus. Building on the concept behind the mobile unit, currently in operation at Mølleåværket, CERE and European partners are to capture CO2 at three industrial sites. One will be stationed at the Portland cement factory in Aalborg, Denmark, while the two others will be constructed at an oil refinery in Romania and at a magnesium-producing plant in Greece.

In Consencus, the partners will go beyond carbon capture and address issues relating to the utilization of the captured CO_2 as raw material. The project will include conversion of CO_2 into higher-value products, and power-based regeneration of the amine solvent.

"Traditionally, solvent regeneration is thermal-based. By switching to power-based regeneration we aim to improve the overall energy efficiency. But obviously, a range of challenges will need to be overcome, since this is an entirely new concept," Philip L. Fosbøl comments.

A truly mobile unit

Increasingly, the field is not referred to as CCS, Carbon Capture & Storage, but as CCUS – with the added "U" denoting "Utilization". Ideally, the captured CO_2 should be utilized instead of being pumped into storage underground. While CO_2 is a culprit in relation to climate change, it is actually attractive for a number of industrial processes and as a raw material.

This philosophy is already in play in the Mølleåværket project. The plant treats waste water from local households with a total of 150,000 inhabitants. The biological components in the waste water are used as raw material for biogas production. The

capture of CO_2 enhances the quality of the biogas. In this way, the carbon capture is not just a cost but also creates value.

The mobile unit can easily be separated into two parts. One is the tower with the absorption and desorption columns. The other is the basic structure with all other equipment. This part has the same measures as a standard container, making transport logistics easy.

The unit was built at Pentair's location in Fredericia. As the unit was moved to Mølleværket, the tower and the base unit were separated, then loaded onto the transporting vehicles, driven across Denmark, and finally assembled again in Lyngby. The entire operation was completed in just six hours.

"We were encouraged to see that we were able to move the unit so smoothly. This flexibility is valuable as the unit has a busy schedule ahead," says Philip L. Fosbøl.

Utilizing CO_2 in water treatment

After its current assignment at Mølleåværket, the mobile unit will be moved back to Fredericia for various technical improvements at Pentair. Then, it will enter into operation at the Amager Ressourcecenter (ARC) in Copenhagen.

The project at ARC is highly ambitious. Firstly, the capacity will be 12 tons of CO_2 per day rather than the current 1 ton at Mølleåværket. And secondly, the captured CO_2 will be utilized in the water treatment in Copenhagen. Consumers will experience a pleasant feeling, when their drinking water becomes slightly sparkling.

"We really need to find ways to utilize CO_2. The average CO_2 emission for a Dane is 7-9 tons yearly. To illustrate, the weight of a large car is about one ton. In other words, we are looking at huge quantities of material. If, for instance, we wanted to use all carbon from CO_2 in production of plastic, no one would have room in their home for that many spoons and knives! Such applications could only be supplementary. For the primary utilizations, we would have to look at applications that utilize CO_2 in large quantities. A promising field is production of synthetic fuels for transportation, another is combining carbon capture with hydrogen-based fuels. Finally, converting power into various fuels and chemicals – also known as Power-to-X or just P2X – will often involve CO_2 as a raw material. We have projects in all of these areas," says Philip L. Fosbøl.

Ample opportunities for students

After the upcoming project at ARC in Copenhagen, another priority will be to move the carbon capture unit to a biogas plant somewhere in Denmark.

"Mølleåværket is a biogas producer. However, production of biogas from sewage water is somewhat different from the typical biogas manufacturing taking place at numerous plants across Denmark, which use pig manure, straw, and other bio-waste fractions as feedstock. We are keen to demonstrate the technology at a more traditional biogas producing facility also," the Associate Professor Philip L. Fosbøl reports.

Several biogas producers have already expressed their interest in hosting the mobile unit. The same goes for some potential industrial partners that emit large quantities of CO_2. It may well be, that CERE and Pentair will have to build more than one mobile unit in the near future.

Assosiate Professor Philip L. Fosbøl & PostDoc Humbul Suleman

Summing up, the carbon capture researchers at CERE have a busy time ahead of them. Fresh hands and heads will be needed. Both students and young researchers interested in the field should expect ample opportunities for contributing.

The carbon capture rocket has truly left its launch site.

Mobile carbon capture unit at the public sewage treatment plant Mølleåværket

Thermodynamic Modelling

Professor Georgios M. Kontogeorgis

Industry takes thermodynamic modelling to heart

Survey: over the last decade, predictive chemical engineering models like PC-SAFT and UNIFAC have increasingly become part of industrial practice. Still, some companies worry that focusing on modelling may lead to young engineers with experimental skills being in short supply.

Originally developed in the academic domain, a number of advanced chemical engineering modelling tools have made their way into the everyday life of the world's leading chemical, petrochemical, and pharmaceutical companies. This is one of the trends seen in a survey initiated by the European Federation of Chemical Engineering (EFCE).

Since the survey is a follow-up to a similar survey from 2010, it is possible to spot changes in industry requirements for thermodynamic and transport properties over the last decade.

"Both optimism and concerns are reported. Some consider that it is now far easier to find and access data than it was 10 years ago. However, as the volume of data production has gone up, the quality of the data has, in some cases, diminished," says Professor Georgios M. Kontogeorgis, CERE, lead author of the study.

Answers were obtained from chemical engineering experts representing 37 companies operating in oil and gas, chemicals, pharmaceuticals, biotechnology, food, chemical/mechanical engineering, consultancy, power generation, software suppliers, and contract research laboratories. The response rate was 60 %, compared to 47 % in 2010.

Models have different advantages

Asked to report on changes since the previous EFCE survey, many respondents mention the increased use of predictive thermodynamic models. Explicitly, the UNIFAC model, cubic equations of state especially in the form of the VTPR (PR using an EoS/GE mixing rule), SAFT especially PC-SAFT, and COSMO-RS are mentioned. Among these models, various companies have different preferences.

"All these models are considered important and highly useful in engineering practice, with VTPR and COSMO-RS appearing more well-known and popular compared to 10 years ago. There is interest in having relatively few models, but the survey participants acknowledge that all models mentioned have their role and application," Georgios M. Kontogeorgis summarizes.

Further, models available in commercial simulators are used more these days. For instance, VTPR is now available in simulators, as well as some high-precision equations of state like GERG2008.

A number of companies state that implementation of PC-SAFT remains a challenge due to standardization issues and that its predictive ability should be further assessed.

Only "exciting" systems find funding

Many participating companies note declining investments in experimental measurements and increased use of molecular simulations, which require experimental verification. Many also mention that the number of experimental groups in academia have declined.

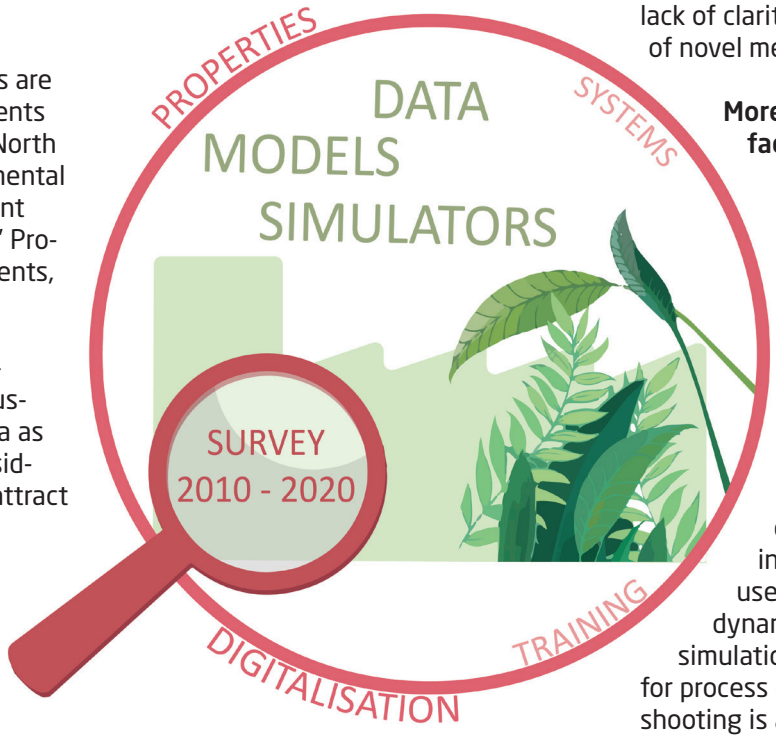
"In our view, the companies are referring to the measurements and groups in Europe and North America, as in Asia experimental activity is not much different compared to 10 years ago," Professor Kontogeorgis comments, continuing:

"For certain classes of mixtures of importance to industry, there is still lack of data as some systems are not considered "exciting" enough to attract government funding."

According to the survey, governments assume that industry should fund property measurements that are always applied or chemicals that are too toxic to be handled in academic laboratories. Thus, while plenty of measurements have been made for vapor pressures and heats of vaporization, similar measurements are needed for more compounds and for a wider range of conditions including high-pressure and high-temperature phase equilibrium data of non-ideal mixtures, data in dilute conditions, cryogenic conditions, and reactive multiphase systems.

Experimental training is neglected

While modelling has become an integrated part of industrial practice, some industry experts worry that the academic world may exaggerate its focus on computational solutions to a degree where experimental training is neglected.



"The university curriculum includes a lot more programming (compared to 10 year ago, ed.), so the new starters are much more versatile in modelling. However, at the same time the experimental skills have decreased, partially due to a priority shift but also due to lack of laboratory space, so we find the time we spent in the past to train up starters in modelling, we are spending now in training starters' laboratory skills," one respondent notes.

Some companies stress uncertainty propagation issues: "the inclusion of model adequacy and parameter uncertainty in thermodynamics could potentially have a major impact on its application in various fields ranging from process to product design" and "the adoption of novel methods is hampered by a number of factors such as clear proof of improvement over existing well-established methods, (lack of) parameterization, and lack of clarity about preferred version of novel method to be used."

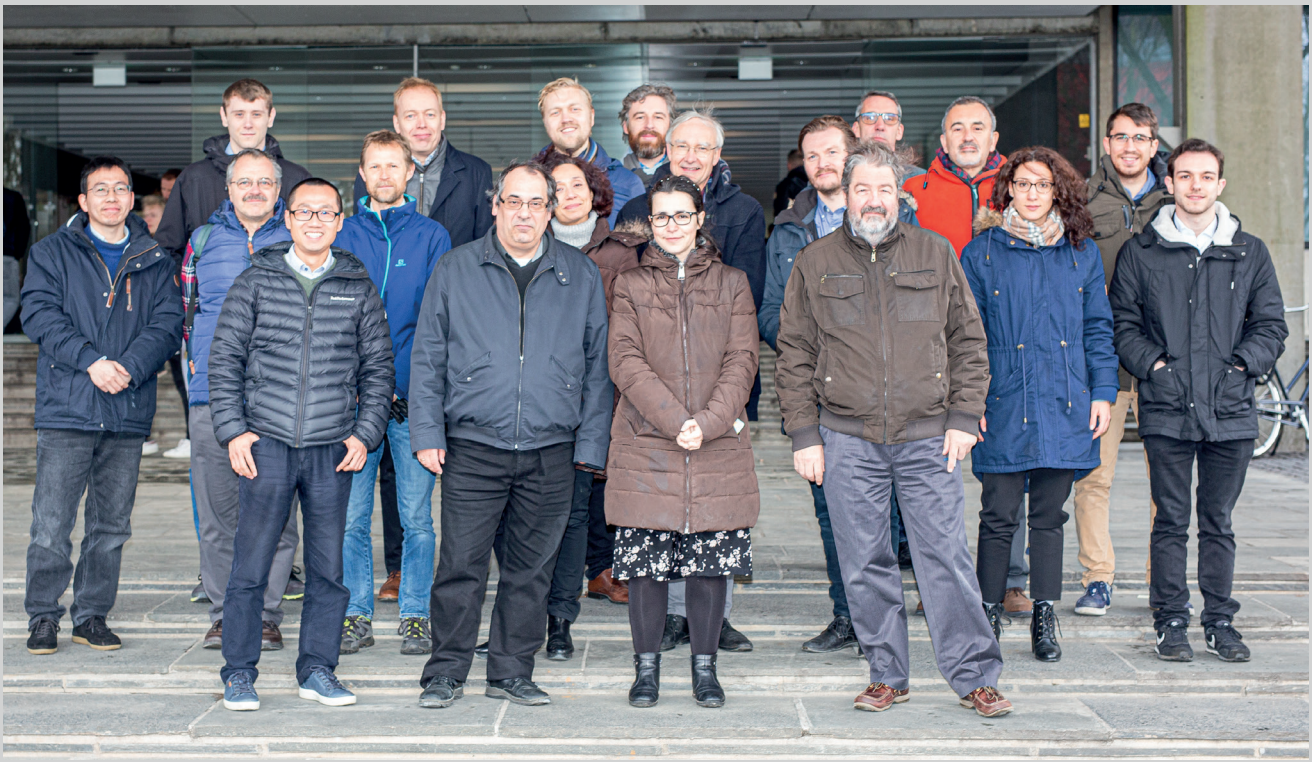
More work needed on interfacial properties

Finally, some companies stress the importance of interfacial properties where more work is needed for both understanding and modelling as well as non-equilibrium thermodynamics, where a better understanding can lead to improvement in process efficiency. The use of computational fluid dynamics (CFD), and numerical simulations in general, as a tool for process development and troubleshooting is also mentioned.

"In this case, there is a need for implementation of more general models and databanks compared to the relatively basic thermodynamics and material models currently used in customer projects," says Georgios M. Kontogeorgis.

The article presents selected highlights from the 2020 EFCE survey. The results are reported extensively in the article "Industrial Requirements for Thermodynamic and Transport Properties: 2020", I&EC Research, American Chemical Society, 2021. Authors: Georgios M. Kontogeorgis, Ralf Dohrn, Ioannis Economou, Jean-Charles de Hemptinne, Antoon ten Kate, Susanne Kuitunen, Miranda Mooijer, Ljudmila Fele Zilnik, and Velisa Vesovic.

European project on modelling of electrolyte systems



The inaugural meeting of the ERC project "New Paradigm in Electrolyte Thermodynamics" took place February 28, 2020 at DTU.

When the European Federation of Chemical Engineering (EFCE) in 2010 asked industry on their requirements, electrolytes were generally mentioned by the respondents as a field that was lacking behind other chemical engineering fields.

In the 2020 EFCE survey, one industrial statement on the subject of electrolytes sounds:

"Electrolytes are more prominent in processes, possibly due to the expansion of bioprocessing. The electrolyte models are more complex than the non-electrolyte ones, and much more difficult to use for practicing chemical engineers. One perceives a lack of standardization when comes to using these models. There is a need for a critical review/comparison/evaluation on these models, similar to what has been done for non-electrolytic models."

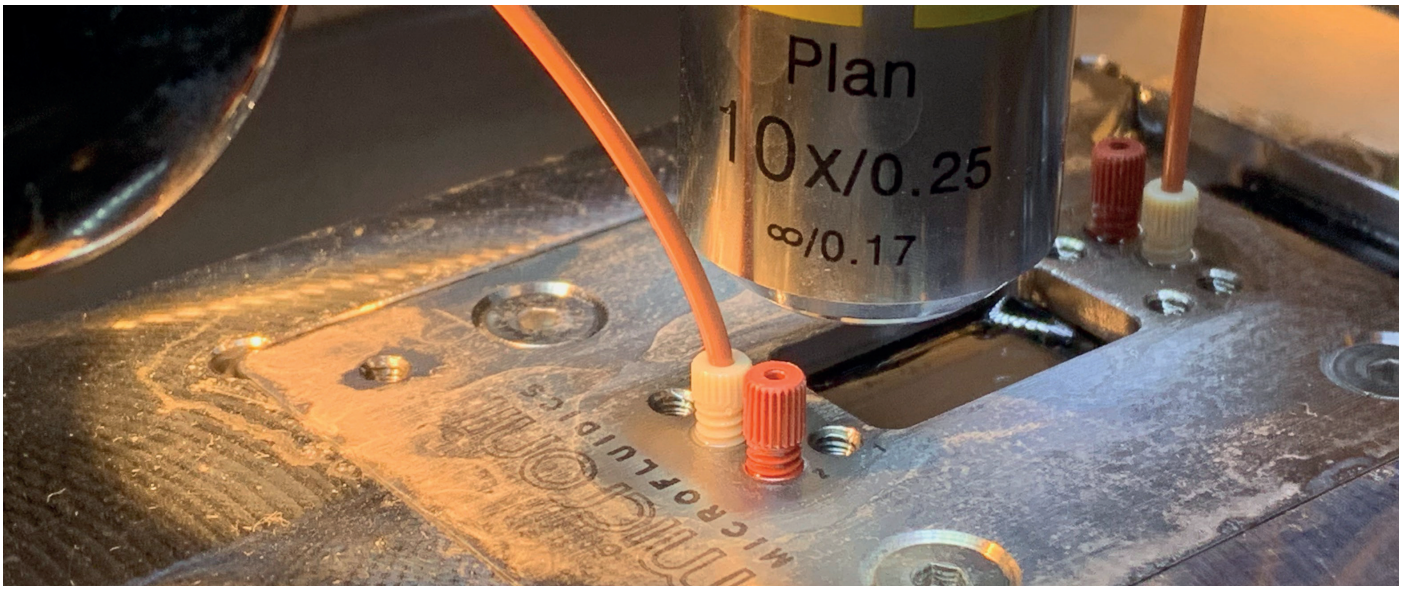
"A large number of companies agree that modelling of electrolyte systems remains a major challenge, both from a fundamental point of view and from a more practical point of view," Georgios M. Kontogeorgis comments. Besides being lead author of the 2020 EFCE study, he is well positioned to make a difference when it comes to meeting the needs expressed by industry on electrolytes. He currently heads a major project funded by the European Research Council (ERC) on "New Paradigm in Electrolyte Thermodynamics".

Besides Professor Kontogeorgis, CERE faculty members, Professor Nicolas von Solms and Associate Professor Xiaodong Liang, have major roles in the project.

Collaborators in the project through the various sub-projects are professors Athanassios Panagiotopoulos, Ioannis Economou, Marcelo Castier, Jean-Charles de Hemptinne and Dr. Bjørn Maribo-Mogensen. Currently 3 PhDs and 4 post-docs are involved, while 1-2 more PhDs will be employed during 2021.

The project was initiated in 2020 and has a duration of five years.

Petroleum engineering



A microfluidics chip under the microscope. The chip is used for the study of coalescence and motion of the oil droplets in the flow.

Top ranking for DTU petroleum engineering

According to QS World University ranking, the petroleum engineering environment at DTU is one of the worlds' finest. Now, an expansion is in the making.

Only National University of Singapore and UT Austin were rated higher than DTU in the petroleum engineering category at the QS World University ranking. Based on some 100,000 expert respondents in the higher education sector, the ranking is the worlds' largest survey of academic opinion. More than 5,000 universities are included.

Institutions are evaluated according to six criteria of which the academic reputation of the faculty is the primary, weighing 40 % of the total score.

"We scored especially high on reputation. Clearly, this was the number one reason we finished as well as we did," says Associate Professor Alexander Shapiro, the Head of studies for the petroleum engineering M.Sc. program at DTU.

Another high-scoring field for DTU was academic citations, weighing 20 % of the total score.

"As for citations, we do have an advantage due to the fact that our program is much more focused on research than many similar programs. Often, other universities will have more emphasis on practical and everyday technical skills," Alexander Shapiro explains.

More flexibility for candidates

Now, wouldn't the prestigious ranking performance encourage DTU to continue walking the current path? Think again!

"We would very much like to expand our current uptake which is, on average, 20 new students yearly. To that end, we are planning to widen our academic field of interest," informs Alexander Shapiro.

Besides petroleum engineering, the study program is to be expanded, to encompass mineral resources in general, geothermal energy, carbon capture and storage, and the environmental side of hydrocarbon exploration such as filtering of production water, minimizing the use of production chemicals etc.

The academic expansion is to a large degree designed to attract more Danish students:

"At the moment, I can only guarantee a Danish student that the oil and gas industry in Denmark will exist for at least the next ten years. What will happen beyond that horizon is

quite uncertain. Therefore, it makes sense to widen the area of interest, providing our candidates with more flexibility."

Adapting to a changed reality

Still, shouldn't a top-ranked university be able to just recruit more international students and thereby compensate for the current hesitation on the side of Danish students?

"We do see large interest from international students, but in a time of global pandemic nothing is straightforward. For students from some of the countries, which traditionally have sent their students to study at DTU, visas are required and this process is largely put on hold because of COVID-19 restrictions. Others experience difficulties due to financial uncertainty caused by the pandemic – they cannot have their stay here paid for," explains Alexander Shapiro, concluding:

"Hopefully, these issues will be solved before too long. But in the meantime, we do everything we can to adapt to the changed reality that we live in!"

Petroleum engineering at DTU

The petroleum engineering activities at DTU take place at several departments: Chemical and Biochemical Engineering, Mechanical Engineering, Civil Engineering, Chemistry, Environmental Engineering, and Compute. Often, research activities are coordinated by CERE. Further, an extensive collaboration with the Danish Hydrocarbon Research and Technology Centre (DHRTC), headquartered at the DTU Campus, exists. Since 2008, DTU has offered a M.Sc. program in petroleum engineering.

From tight to extremely tight chalk

A large part of the Danish oil and gas reserves are in geological formations, which challenge academic understanding of the mechanisms involved in oil production.

Oil and gas production in the Danish part of the North Sea has to date been mostly concentrated on the younger Upper Cretaceous layers. However, also the Lower Cretaceous layers contain substantial oil and gas reserves, some of which are being produced now. Several ongoing projects in CERE, all undertaken in collaboration with and sponsored by DHRTC, focus on these deep and complex reservoirs.

A key question relates to the composition of the oil in a Lower Cretaceous reservoir. Traditionally, the oil of an oil reservoir is regarded as having the same composition all across the reservoir (but not along its depth). Since the reservoir was formed millions of years ago, any original differences in composition are assumed to have been levelled out. In chemistry terms, the reservoir is said to be in equilibrium. However, in extremely tight carbonate reservoirs it can be imagined that even during all this time, oil with different compositions has been unable to fully mix due to very long mixing times and internal barriers in the reservoir.

"This is an ongoing debate. Indeed, samples taken from different places in extremely tight reservoirs have indicated that the oil could actually be not in equilibrium. However, recent results from our research suggest that the problem could lie in sampling errors. Accounting for the temperature differences levels out the oil compositions in horizontal direction," says Associate Professor Alexander Shapiro, heading the petroleum engineering research at CERE.

Making the most of scarce samples

The problem is addressed in the PhD project of Hadise Baghooee at CERE. Project partners are DHRTC, University of Pau (France) and energy corporation Total. Headquartered in France, Total acquired the former Maersk Oil and is today the main operator in the Danish part of the North Sea.
A key challenge in this type of research is the scarcity of the reliable samples
The research is focused on the Valdemar Field which is believed to contain the largest amounts of oil among the Lower Cretaceous fields in the Danish part of the North Sea. Careful analysis of the samples taken at different depths, carried out by Hadise Baghooee, suggest that the Valdemar Field does indeed have an internal barrier separating the higher and lower parts of the reservoir.
"What we have seen in the project of Hadise Baghooee is that the differences in the samples could actually have been introduced when the samples were taken. Since oil and gas do not flow at the same rates, there is always a risk that you do not get the

Cleaning of water is a part of modern oil production

Offshore production of oil and gas will always have water as a by-product. In a Danish context, the offshore reservoirs contain a lot of water, which is produced together with the oil in, at least, equal amounts. Extensive application of waterflooding increases this production. In recent years, an important focus of the DHRTC-CERE collaboration has been to improve the environmental properties of the produced water by removing both oil residues and other forms of pollutants.
"The produced water can either be re-used, so injected back into the reservoir as part of the ongoing water flooding, or discarded into the sea. In both cases, the water needs to be cleaned as it contains various impurities such as oil drops, solid particles, corrosion inhibitors and other chemicals," explains Associate Professor Alexander Shapiro, CERE.
In a project of Postdoc Liridon Aliti, cleaning of water with application of the different chemical reagents is investigated. A novel experimental technique, microfluidics, is applied for this study. The water containing the generated oil droplets is flowing in tiny capillaries. The process is studied under microscope and captured by a high-speed camera. Coalescence (merging) of the droplets is observed, and right concentrations of the chemicals promoting the coalescence are selected. Ideally, this should result in formation of the larger droplets, which are much easier to remove. The project is supervised by Advisor Simon I. Andersen, DHRTC, and co-supervised by Alexander Shapiro.

true oil/water composition when you take the sample," Alexander Shapiro explains.

Non-trivial theoretical questions

Notably, samples taken at different depths will also be taken at different conditions of pressure and temperature, which again might lead to systemic differences in the oil/water composition errors – giving the false impression that the reservoir is not at equilibrium.

"Seemingly, corrections on the gravity and temperature can explain the observed differences, and the oil in the Valdemar Field is indeed in equilibrium," says Alexander Shapiro, adding that the project turned out to be more challenging than assumed beforehand:

"The project involves some non-trivial theoretical questions. Try to think of the heater in your house. Probably you have noticed that the heater has a tendency to attract dust. Something similar goes on in a reservoir: the heavier oil components will have a tendency to move towards the warmer parts of the reservoir. However, the quantitative evaluation of this effect, called thermal diffusion, is very difficult to obtain. It must be evaluated properly to get the correct picture. We have collaborated with the researchers from the University of Pau, France, who suggested a new theory for thermal diffusion. The theory was validated for other reservoirs from the North Sea, and then applied to Valdemar."

Gas bubbles threaten production

Another research topic is related to the oil production from Valdemar. This reservoir is produced by depletion, where pressure decreases when the oil is produced. A known obstacle here is the solution gas being liberated from the oil in the form of gas bubbles due to the decline in reservoir pressure. These gas bubbles threaten further oil production as they will tend to fill the tight porous space, lowering the oil's mobility. A Ph.D. study of Wael Al-Masri performed in collaboration between CERE and DHRTC has studied this effect, both in modelling and experiments. The project demonstrates that just 10 % of the gas liberated is enough to cause a 75 % decrease in oil flow velocity.

"To mitigate this effect, industry tends to maintain the pressure above the bubble point by injecting water or gas into the reservoir. However, this is not always possible. Often, the best way to extend a flooded reservoir's life in terms of cost, ease of implementation, and environmental impact, is depressurization below the bubble point," explains Alexander Shapiro, supervising the project.

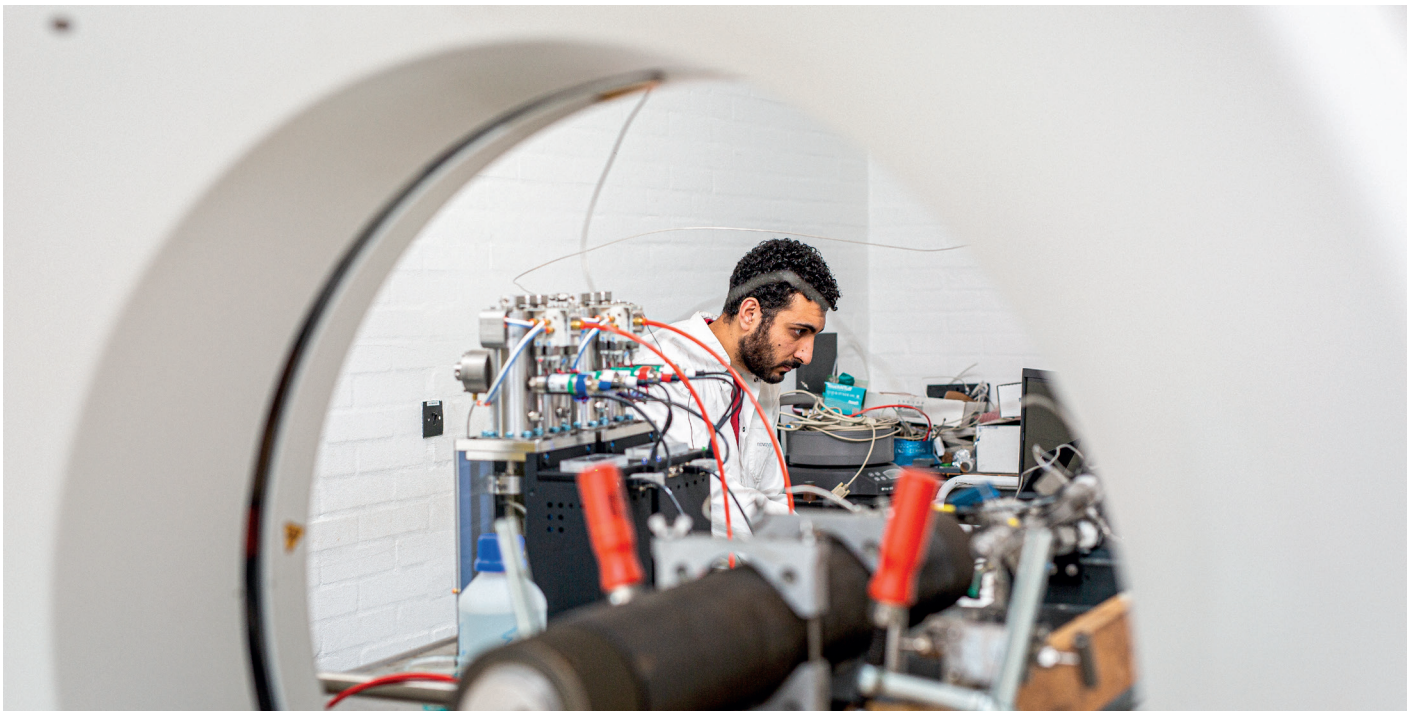
"Rather than trying to avoid gas bubbles being formed, a better idea might be to increase the formation so fast that the bubbles will begin to flow instead of plugging the porous media," says Alexander Shapiro.

A difficult process to mimic

During the experiments, pressure is gradually decreased from above to below the pressure at which gas forms. The oil mobility is estimated by injecting oil through the rock sample and measuring the pressure difference needed for the oil to flow through the rock sample. X-ray computer tomography is applied to measure the amount of trapped gas. The process is repeated until the gas becomes mobile and exits the sample. At this point, the maximum amount of trapped gas is measured.

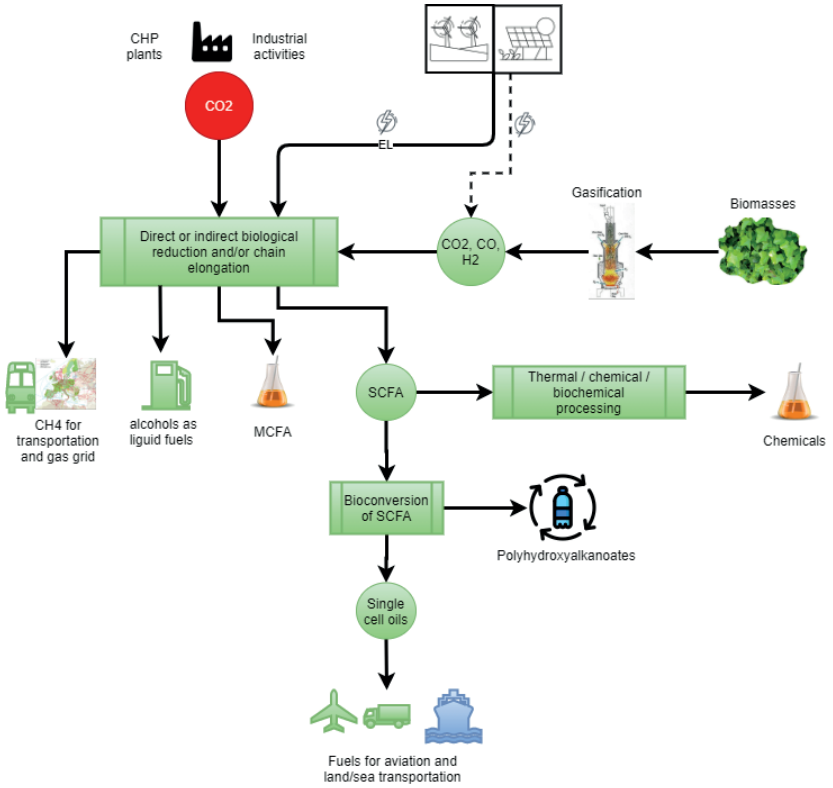
"Mimicking this process in the lab is really challenging. Wael Fadi Al-Masri is one of the first researchers in the world to have achieved this," notes Alexander Shapiro.

Presently Wael continues as a postdoctoral researcher at CERE, supported by the DHRTC. In the ongoing research, he investigates new approaches to tackle the issue of bubbles.



Postdoctoral researcher Wael Al-Masri working on the experiments on gas liberation from oil in the rock of a petroleum reservoir, with the application of X-ray computer tomography

Valorization of gases



Flow chart for biological valorization of gases. Starting from biomasses (top right) and carbon dioxide in industrial off-gases, a range of different end products can be produced. MCFA denotes Medium Chain Fatty Acids, while SCFA are Short Chain Fatty Acids.

CO_2 and syngas as production platforms

Fermentation of syngas and similar biological processes have emerged as attractive, green methods for production of fuels and chemicals. The first industrial breakthroughs have come, and research into ways to increase yields and optimize economic feasibility for a range of products continues at high pace.

In 2018, Lanzatech inaugurated a plant in Caofeidian, China, using syngas from a steel mill as feedstock for production of ethanol. While syngas - a gaseous mixture of mainly CO, H_2 and CO_2 – has previously been utilized for fuel or chemical production on various occasions throughout the history of industrialization, this plant is different as the core production process is fermentation. The capacity of the plant is 48,000 metric tons ethanol per year.

"This was the first commercial scale plant to use syngas fermentation for production of ethanol. A wide range of other plants using the same or similar technology are in pilot or demonstration phases. This reflects how both industry, academia, and policy makers increasingly take interest in biological valorization of gases," says Hariklia N. Gavala, Associate Professor, CERE.

Biological methods for gases valorization come with certain advantages over chemical catalytic processes. The biocatalysts (microbes) present a higher tolerance to impurities, operate at mild temperatures and pressures, which results in significantly lower operating cost, have higher product specificity and do not require a fixed C/H ratio. Further, they open new routes for production of high-value chemicals.

CO_2 as a valuable raw material

A range of waste products from agriculture, forestry, and food industry can be gasified. The same goes for municipal solid waste which is

generally difficult to utilize due to the high variability. Even plastics waste – a rapidly growing type of waste – can be gasified.

"The high transformation efficiency of the feedstock carbon is a really attractive feature of gasification and further biological processing. In addition, concerns about pathogens, which is very often the case for sludge and animal wastes disposal are eliminated this way," says Hariklia N. Gavala.

Known as Fischer-Tropsch synthesis, transformation of syngas into liquid fuels and chemicals has been a well-established technology since the 1920's. The method is relatively costly due to low energy-efficiency, but has been used in some scenarios. For instance, when liquid fuels were scarce during the second world war, coal was gasified to produce liquid fuel for vehicles.

However, biological routes for the conversion were not investigated until quite recently. It was just towards the end of the 20th century that the scientific community became fully aware of the metabolic features behind CO_2 and CO fixation by acetogenic prokaryotes. This realization opened the door to a new type of biochemical engineering in which CO2 was not just seen as a problematic greenhouse gas but also as a potentially valuable raw material.

Production of ethanol was the first wave

The first wave of interest centered itself around production of ethanol. This was in-line with the intense efforts for finding ways to produce sustainable and renewable liquid fuels towards the end of the 20th century. In the last two decades, interest has widened to include production of methane and a number of other chemicals and materials like longer chain fatty acids, alcohols, and platform chemicals such as short chain fatty acids, which can be used as precursors of a number of interesting products including polymers such as poly-hydroxy-alkanoates (PHA).

In several ways, syngas biological conversion processes are similar to processes that have carbon dioxide and hydrogen as production platform. Both microbial systems rely on the reductive acetyl-CoA pathway for assimilation of CO_2 and, in the case of syngas, CO.

"The low solubility of compounds acting as substrates for the microbial growth – CO and H_2 – resulting in low mass transfer rates and low microbial growth rates, and consequently in low production rates, is the main challenge in both cases," says Hariklia N. Gavala.

Smarter reaction designs

At CERE, Hariklia N. Gavala heads long-standing efforts to improve the efficiency of microbe-based chemical engineering:

"Intensification of the bioprocesses of both syngas and carbon dioxide will be a necessity for reaching technological maturity and economic feasibility. We have shown that reactors based on attached growth may enhance conversion rates through high concentrations of cells, while smart designs such as trickle beds allow for enhanced mass transfer rates. In this way, it will be possible to avoid operating at increased pressure, and thereby also avoiding high operating and construction costs, and toxicity problems. We have also shown a potential for increasing the productivity of the system by several folds."

Besides smarter reactor designs, a major effort in the group is development of consortia of microorganisms optimized for the task. There is a trade-off between using customized microorganisms for a given task or mixed consortia. The tailormade microorganisms generally give higher yields, but also imply higher costs, increased sensitivity to inhibitors and lower stability in continuous systems. Originally, mixed consortia known from environmental technology were used, but recently more specific blends have been developed.

"The stability and reproducibility of processes based on mixed communities need to be further investigated so they become attractive for industrial applications. Strong evidence suggests that such processes can indeed be stable and reproducible," says Hariklia N. Gavala.

The yield versus productivity trade-off

"Yield versus productivity is a more challenging issue for gas bioconversion processes compared to traditional liquid-based processes. Careful considerations and analysis are required before deciding on production microorganisms and reactor systems."

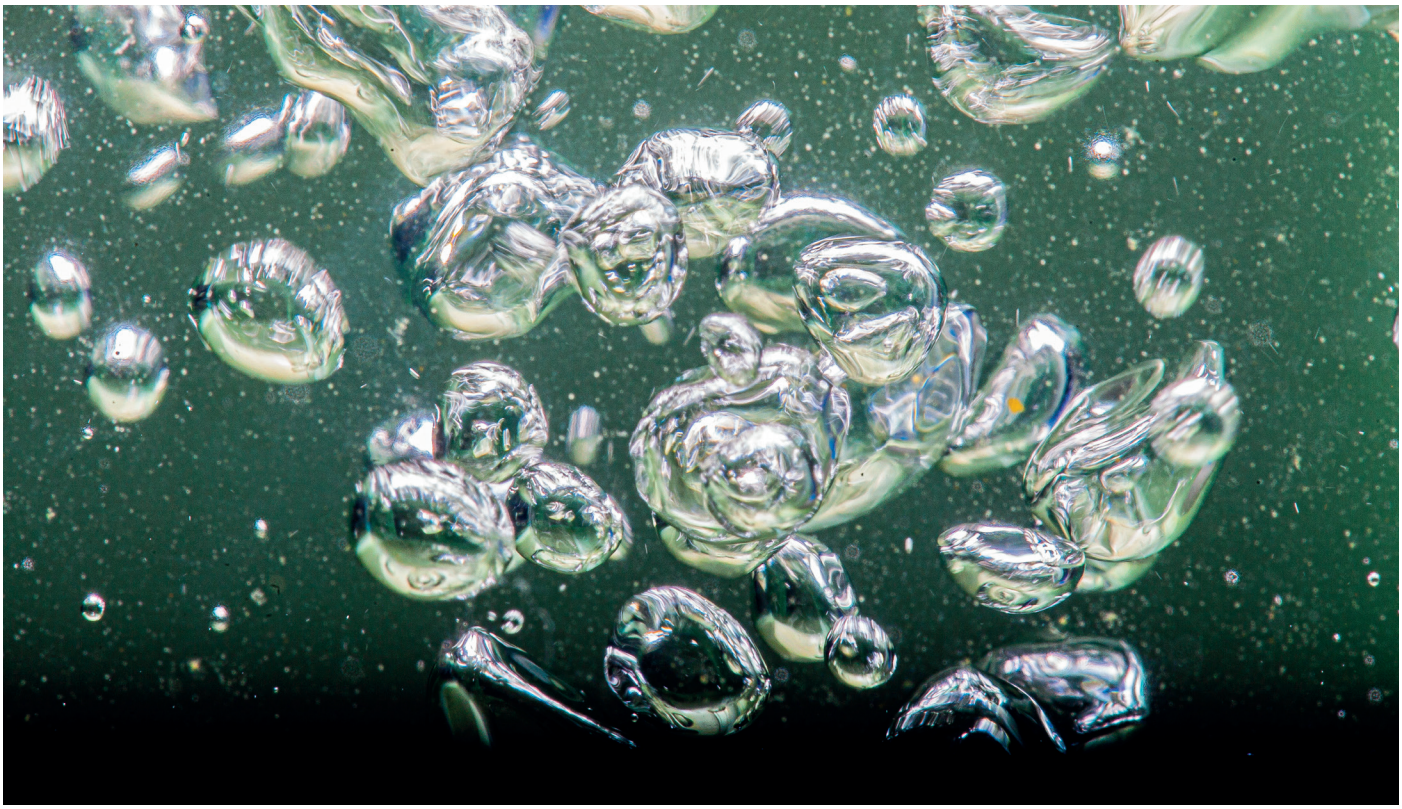
A further challenge for these emerging technologies is to compete with existing petrochemical industry due to the currently low price of fossil fuels.

"We and other research groups work hard to remove existing bottlenecks in CO_2 bioconversion and optimize bioreactor configurations for maximum productivity. However, some assistance from governments will be essential to achieve global decarbonization and reduce the negative effects of carbon emissions," says Hariklia N. Gavala, adding:

"Political stakeholders should enhance incentives for upscaling of CO_2 capture and utilization bioprocesses. For instance, a carbon footprint fee or a substantial reward for negative CO_2 emissions could speed up the commercialization of bioenergy production units."

Associate Professor Hariklia N. Gavala

Water



if we want to understand bio molecular communication, we have to look at the dynamics of bio molecule hydration and how water behaves at surface interfaces

When proteins communicate through water

The docking of one bio-molecule to another may be preceded by electromagnetic communication. A new project at CERE will investigate the interaction.

In pharmaceutical contexts, the binding of the active drug to its target protein is often described as a hand fitting into a glove. However, this docking event may be preceded by communication between the two molecules. A highly ambitious project at CERE is set to investigate the phenomenon.

"In the field of drug discovery, people always have the respective structures of the drug candidate and the receptor molecule as their main focus. How well do the two molecules fit? However, it is well established that a high degree of intermolecular vibration is involved. We want to investigate if these vibrations are in fact modified in a way that helps to facilitate the docking. If so, the implications could be relevant in a wide range of pharmaceutical and other applications," says Michael Bache, Senior Researcher, CERE.

He comes from a microfluidics background, and joined CERE when a water research group was founded some years ago.

"The fundamental behavior of water molecules has always been at the center of my research. This is also true for this new project. If indeed bio-molecules communicate in the way we imagine, it could be through water. Therefore, the behavior of water will be a key part of the investigation. Not least the behavior of water at the liquid-solid interface which is also a core focus in microfluidics," explains Michael Bache.

Femtosecond chemistry

The opiate dermorphin is chosen as the primary research subject. The molecule exists in two versions with one chiral group difference – D-Alanine vs. L-Alanine. Although similar in structure, only the D-ala form has activity.

The group at CERE has shown that the two chiral versions differ in infra-red absorbance and only when in water. In the new project, the structure of the dermorphin mu-receptor molecule and their corresponding chiral molecules will be investigated. Since the two forms are structurally similar, a hypothesis would be

that the very different effect in a biological system – for instance the human body – could be attributed to differences in vibrational behaviour in water.

The group will build a graphene flow cell able to separate ligand from receptor while still allowing electromagnetic communication. As molecular processes take place at extremely high speed – in femtoseconds, 10-15 seconds - it is necessary to study them in a soft matter X-ray synchrotron facility. The group is working on getting beam time at the DESY synchrotron, Germany.

"We propose to use a flow cell to physically separate the dermophine peptide from the receptor. The membrane will consist of an atomic monolayer of graphene, since it is transversely electrically conductive for electromagnetic communication effects and has a high membrane strength," says Michael Bache.

Opening new doors in water research

The upper part of the flow cell will contain the mu-receptor while the lower part the two different enantiomers of D and L dermorphin. The effect on the mu-receptor will be analysed in-line using X-ray soft matter synchrotron spectroscopy, showing how water is behaving around the molecules.

Parallel to the experiments, the group will continue classical spectroscopic and theoretical investigations on the docking process of ligands onto a mu-receptor molecule, performing quantum and classical calculations of the structure and computer simulations of the docking process.

"We are hoping for a dual outcome. Firstly, we want to investigate the molecular interactions involved in this specific process. Secondly, we hope to expand the use of femtosecond X-ray investigations for this type of phenomena which could open new doors in other aspects of water research."

The project "Study of electromagnetic communication between chiral drug molecules and its receptor in water" has been received two million DKK as an Villum Experiment grant from Villum Fonden. The project will begin June 2021 and have a duration of two years.

New project on water structure and properties

Despite the simplicity of a single water molecule, the world's most important liquid remains a hot research topic. The new project WATSIM at CERE aims to investigate how models, simulations and theories can help in understanding the structure and properties of water under different properties.

"Water plays an essential role in almost all science and engineering disciplines," says Associate Professor Xiaodong Liang, heading WATSIM.

"It is also believed that the hydrogen-bonding plays a central role in understanding water. The nature of the hydrogen-bonding network in liquid water continues to be at the center of the scientific debates."

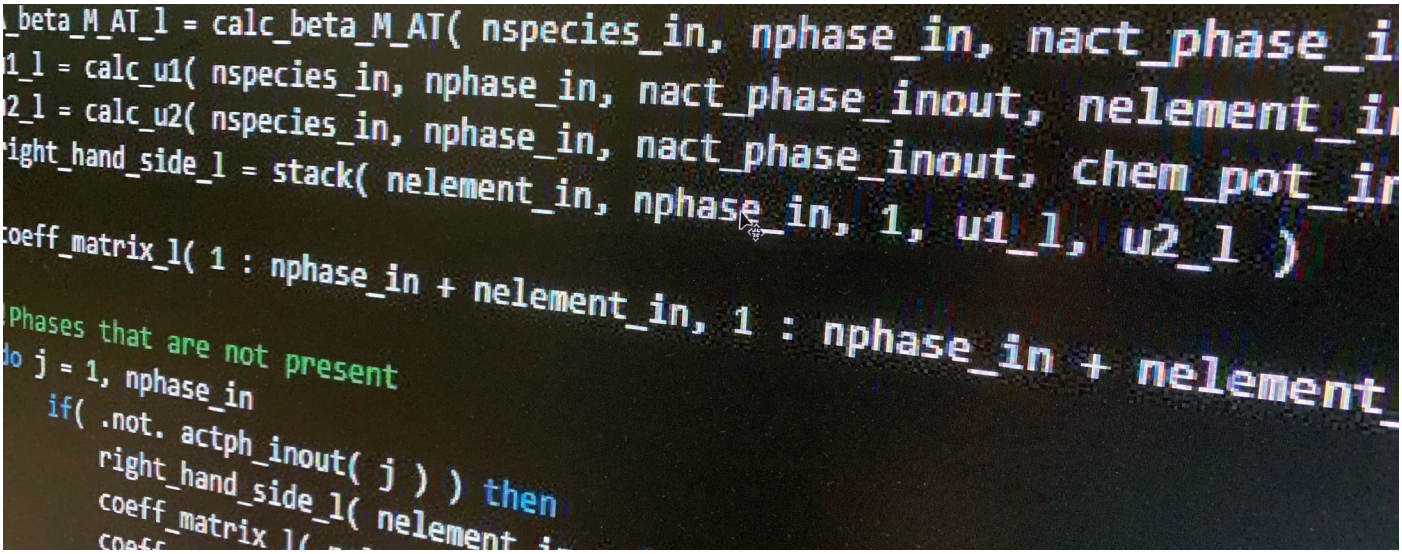
The project aims to study the structure and properties of water over a wide range of temperature and pressure, confined in porous media/ nano-particles, from molecular simulations and thermodynamic theories.

One PhD project and one Postdoc project are included in WATSIM. Aswin Vinod Muthachikavil will investigate "Water structure and properties from molecular simulations and Yuan Chen has worked on "Ab initio molecular simulations for water."

WATSIM has a duration of three years. The project has been made possible by funding from PetroChina. It has a close collaboration with the PhD project of Evangelos Tsochantaris "Advanced thermodynamic models for water" which is part of the ERC Advanced Grant project "New Paradigm in Electrolyte Thermodynamics".

Senior Researcher Michael Bache

Flash Calculation



Robust and efficient flash code provides the engine for dynamic simulation of chemical and subsurface processes, often with multiple phases and reactions.

Applying flash calculations to open systems

CO_2 sequestration and production of shale reservoirs are just two of many chemical engineering problems which new algorithms developed at CERE can help to solve.

A common phenomenon at any plant producing or treating fluids is spontaneous evaporation taking place due to pressure drop when the liquid stream passes through some kind of confinement such as a throttling valve. This is known as flash. In industry, accurate flash description is imperative since uncontrolled evaporation could be highly hazardous. Relevant algorithms for industrial applications have been around for a long time. Now, a team at CERE has shown that it is possible to extend the use of flash algorithms for a range of other environments.

"Currently, we are applying our methodology in a study on CO_2 sequestration, and we understand that they would also be valuable for instance in production of shale reservoirs," says Associate Professor Wei Yan, CERE.

Phase equilibrium calculation is essential to process simulation in many engineering disciplines and scientific areas, such as chemical engineering, petroleum engineering, mechanical engineering, and geo-chemistry. The calculation determines the distribution of species between equilibrium phases, and it is often coupled with mass and energy balances for process analysis and design.

Three types of equilibrium problems

At an industrial plant, flash evaporation will typically take place in a closed system. For instance, a throttling valve would be located at the entry into a pressure vessel, so that the flash evaporation occurs within the vessel. This is called a flash drum.

"The term flash is traditionally used for separation in a flash drum or a similar closed system. What we have shown is that it is possible to develop algorithms at the same level of robustness and efficiency for open systems," says Wei Yan.

The new methodology is published in the prestigious AIChE Journal, American Institute of Chemical Engineers. Authors are three CERE scientists, PhD Student Fernando de Azevedo Medeiros, Professor Erling H. Stenby, and Associate Professor Wei Yan. Also recognized should be Professor Michael L. Michelsen (1944-2020) whose many groundbreaking contributions to the field of flash calculation is the foundation for the work.

Michael L. Michelsen classified the equilibrium calculation problems into three types: flash specifications leading to thermodynamic state function minimization; phase fraction specifications; and other specifications. The first type refers to isothermal (TP)

flash, isenthalpic (PH) flash, isentropic (PS) flash, and so forth. The second type is represented by saturation point calculation, but the specified phase fraction can also be a value between 0 and 1. The last type includes somewhat exotic specifications like (P,V) and (T,H) and indirect specifications like critical point calculation. Among the three types, only the first type always corresponds to a unique minimum of a thermodynamic state function, and can thus be solved in a robust manner with the help of stability analysis. Among all the flash specifications, TP flash is the most widely used and has well-developed algorithms especially for two-phase calculation.

Q-function approach extended

A defining feature of Michael L. Michelsen's contributions was his commitment to minimize the number of calculations in order to save computing resources and thereby reduce costs and increase the practical value of the methodology. To that end, he introduced so-called Q-functions – a Q-function is the tail-end of the standard normal distribution – into a range of flash calculations.

In the new study, Medeiros, Stenby and Yan have analyzed the Q-functions suggested by Michelsen for state function-based flash specifications.

"We showed that a Q-function relates the thermodynamic state function to be minimized for a flash specification and the state function whose natural variables are used in the flash formulation. A paper by Michelsen essentially described how to perform state function minimization in (T, P, n) based thermodynamics or (T, V, n) based thermodynamics," Wei Yan explains.

"Based on the analysis, we extended the Q-function approach to open systems. For an open system, it is possible to define a state function to be minimized. We categorized the corresponding equilibrium calculation through minimizing the state function as the flash-type calculation. New Q-functions can be introduced to solve the flash problems for open systems."

Systems with and without reactions

Not only does the methodology work for open systems, it can even be applied both to systems with reactions and to systems without reactions.

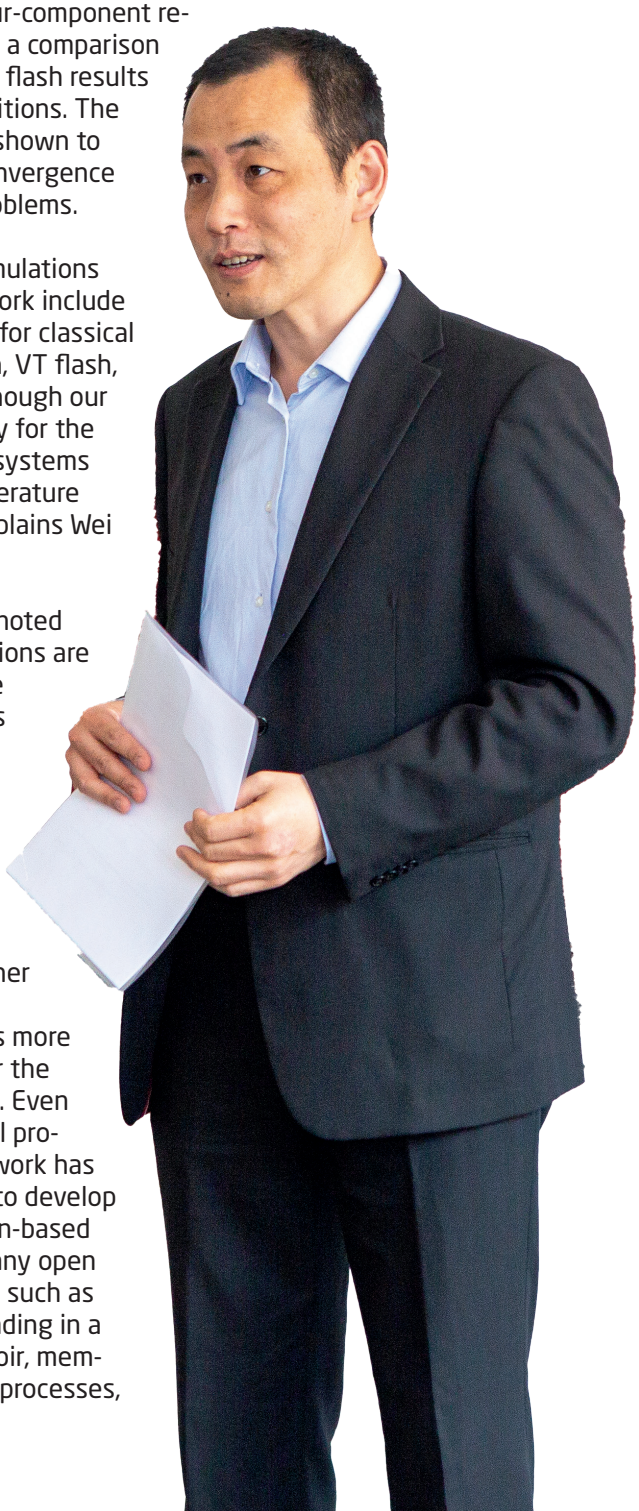
"For open systems without reactions, we suggest Q-functions and a formulation using the classical framework, with the mole numbers as independent variables. For open systems with reactions, we suggest Q-functions and a formulation using the recently proposed RAND framework," says Wei Yan.

To validate the algorithms, the CERE team applied Q-function minimization to a non-reactive hydrocarbon mixture and a four-component reactive mixture by a comparison with the classical flash results at the same conditions. The algorithms were shown to give quadratic convergence for the tested problems.

"The general formulations provided in our work include the counterparts for classical PH flash, PS flash, VT flash, and UV flash, although our examples are only for the two-phase open systems at constant temperature and pressure," explains Wei Yan.

It should also be noted that the formulations are not limited by the number of phases either.

"In principle, the formulations lay out the basis for robust and efficient algorithms for other types of flash, although it requires more detailed study for the specific problems. Even for the isothermal processes only, the work has made it possible to develop more minimization-based algorithms for many open system problems, such as compositional grading in a petroleum reservoir, membrane separation processes, and geochemical calculations," Wei Yan concludes.



Associate Professor Wei Yan

News from CERE

Professor Nicolas von Solms

New CERE chairman

Two career milestones were reached simultaneously by Nicolas von Solms in 2020, as he was appointed full Professor at DTU in October and then, in November, succeeded his colleague Georgios M. Kontogeorgis as CERE chairman.

"It is a great honor and responsibility to take over the leadership of a center with such a long and storied history. I hope to continue the excellent work done by my predecessors," Nicolas von Solms said, continuing:

"The CERE industrial consortium is one of our greatest strengths and the connection to international industry has been a hallmark of the center ever since its inception in the 1980's. As chairman I will continue this tradition – consolidating and strengthening collaboration with our Consortium members."

"Naturally we will continue to provide a high level of service to our member companies – software, access to publications, experimental data, and discussions on research directions. Another CERE characteristic is the cross-disciplinary academic profile, spanning across several departments at DTU – Chemical Engineering, Chemistry, Compute, Civil Engineering, and Space.
"This unique construction enables an interdisciplinary approach to solving large problems – an approach which is necessary for example in Carbon Capture Utilization and Storage (CCUS), an area where I plan to initiate one or two larger projects across the departments."

Nicolas von Solms joined DTU in 2001, first as Postdoc, then since 2005 as Associate Professor. His main focus was always chemical engineering fundamentals, especially applied thermodynamics used e.g. in relation to CCUS, flow assurance and materials.

Group picture from 2019

Course on advanced thermodynamics went online

The global COVID-19 pandemic was unable to put an end to a longstanding tradition at CERE: The summer course on advanced thermodynamics was initiated by Professors Michael L. Michelsen and Jørgen Mollerup 25 years ago, and has been given by them and other CERE faculty members ever since. The 2020 version of the course took place in an online form during two weeks of August 2020. Associate Professor Wei Yan was overall organizer with assistance from other faculty members and – for the exercises – PhD students.

Dr. Matthew Jones, Shell Projects & Technology, participated "as a relative newcomer to the field, but very interested to learn more, after working on projects supporting operations at LNG plants."

"The course was very impressive, covering computational methods in great detail, while also giving a good overview of the different types of models in use for a wide range of different applications. I feel like I learned a great deal over the two weeks," he says.

According to Matthew Jones, the adaptation to the online format was successful:
"I found that having access to the lecture videos allowed me to take the material at a speed that was right for me, and the presenters were always ready to answer any questions that we had. I'm now looking forward to being able to apply the things I learned to projects within Shell, and to continue to explore the topics."

Obituary of Professor Michael L. Michelsen

Professor Emeritus Michael L. Michelsen passed away on 26 August, 2020.

During four decades, Professor Michelsen was a world-leading authority on thermodynamics, and in particular on the development of algorithms for the efficient and fast computation of phase equilibrium for non-ideal mixtures.

He developed numerical procedures for multi-component, multi-phase phase equilibria, which is the typical situation in practice (industry and nature). Such algorithms are of paramount importance for the design and operation of complex processes and they have found widespread use in the chemical and petroleum industry.

Professor Michaelsen also showed how enhanced understanding of the mathematical interrelations can result in new advanced models and opportunities. For example, he pioneered the development of advanced mixing rules for cubic equations of state and thus showed how the classical solution models, originally developed for low pressures, can be employed at higher pressures of interest in many industrial applications. Later, Michael L. Michelsen showed how the newly developed association models (for mixtures with complex interactions like hydrogen bonds) can be formulated in ways that permit their efficient implementation and use for challenging applications.

Always, Professor Michelsen remained at the forefront of science, continuously following the developments and contributing not just to thermodynamics but to a large variety of disciplines. He made significant contributions especially in relation to numerical methods in fields like reaction engineering, transport phenomena, and material science with emphasis on polymer solution thermodynamics.

A worthy successor of thermodynamic giants (and Nobel Prize winners) van der Waals (1910); Debye (1936); L. Pauling (1954): Lars Onsager (1968); Paul Flory (1974); Ilya Prigogine (1977), Kenneth Wilson (1982); Walter Kohn and John Pople (1998), professor Michelsen's algorithms contributed to bringing thermodynamics into the modern era of computational tools, profoundly changing engineering practice.

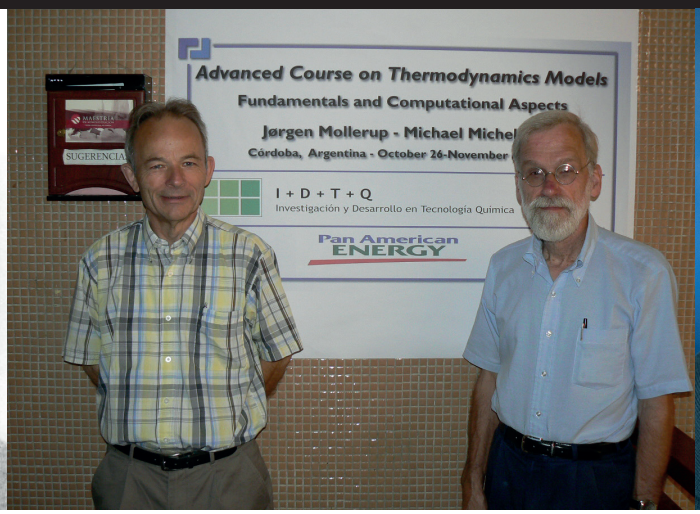
Michael L. Michelsen published about 150 scientific articles and co-authored three books. In particular, the most recent book (co-authored with Jørgen Mollerup) became the basis of a PhD course, which they started 25 years ago. The course is still taught every year in August by current CERE faculty members.

Professor Michelsen will also be remembered by his students as an excellent teacher. He was always willing to help, while at the same time being demanding, setting high expectations.

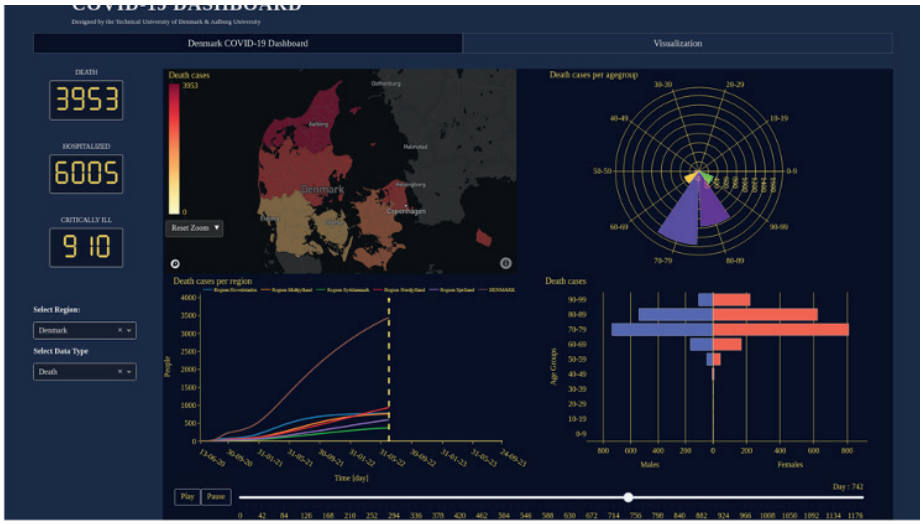
Michael L. Michelsen retired from DTU by the end of 2012, but continued as an active Emeritus until the end of his life. His last co-authored manuscripts are in the process of being published in the journal Fluid Phase Equilibria.

The contributions of Michael L. Michelsen will continue to impact chemical engineering thermodynamics globally for many years to come. His scientific spirit and inspiration will remain at CERE. His genius and great personality will be deeply missed.

Professor Michael L. Michelsen (14 February, 1944 – 26 August, 2020)



Decision support for managing an epidemic



Closing down society was an immediate response to the COVID-19 pandemic, but on the longer haul more sophisticated strategies are needed.

Professor John Bagterp Jørgensen

Associate professor Allan P. Ensig-Karup

CERE faculty members, Professor John Bagterp Jørgensen and Associate Professor Allan P. Engsig-Karup, are involved in a project to this end.

The project, which is a DTU/Aalborg University collaboration, develops a new mathematical decision support tool for the Danish authorities. The aim is to limit the spread of COVID-19 so as to shorten the epidemic, without straining the health care system beyond its critical capacity in terms of number of intensive care beds, ventilators, etc. This will be done through mathematical modelling, simulation, control and optimization in relation to various possible interventions and measures available to the authorities, such as restrictions on social gatherings, close of institutions, isolation of potentially infected individuals and isolation of vulnerable citizens.

The models will be calibrated on a continuous basis and will thus utilize information data from hospitals etc. as soon as these data become available. The developed tool will enable the authorities to select the optimal combination of interventions and their duration. The tool also describes how to establish a gradual and controlled reopening of society.

The project is financed by the Novo Nordisk Foundation emergency coronavirus program.

Busy year for carbon capture PhD

PhD Student Jyoti Shanker Pandey, CERE, began 2020 by attending the 4th International Workshop on Offshore Geologic CO_2 Storage, February 11-12 in Bergen, Norway. Soon after, most countries went into COVID-19 lockdowns, turning conferences and workshops into online events.

At the Interpore 2020 conference, held online August 31 to September 4, Jyoti Pandey gave two presentations and received the conference grant. Furthermore, he attended the AGU20 Fall meeting, held online December 1-17, and the Society of Petroleum Engineers (SPE) Virtual Europec Conference December 1-3.

During the international events, Jyoti Pandey provided several contributions.

Poster: Low Dosage Chemical Assisted Enhanced CH_4 Production and CO_2 Storage in Porous Medium during Hydrate Swaping.

Presentations: Methane hydrate formation, storage and dissociation behavior in unconsolidated sediments in the presence of environment-friendly promoters; Visualization of CH_4 hydrate dissociation under permafrost temperature conditions using a high-pressure micromodel.

PhD student Jyoti Shanker Pandey

PhD

Oil Production Estimation for Fractured Reservoirs

Justin Brand Ferrell, PhD.

Currently with DeGolyer and MacNaughton.
Full title: "Estimation of Matrix Flow Contribution in Naturally Fractured Reservoirs".
Supervisor: Alexander Shapiro.

Naturally fractured carbonate reservoirs (NFRs) account for more than 60 % of the world's proven oil reserves. Estimations of future production from NFRs tend to be less accurate than for single porosity reservoirs. Future production will typically be overestimated, possibly leading to billions of dollars of lost investment to host governments and corporate shareholders. In the project, methodology for higher accuracy in estimations relating to NFRs was developed.

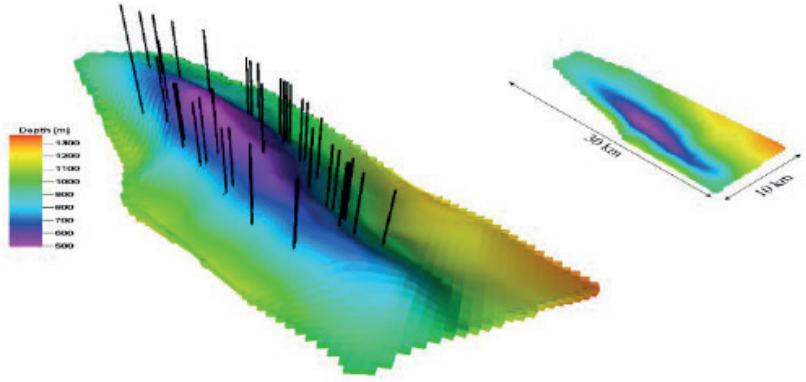
A vast majority of the world's conventional oil reservoirs are naturally fractured (NFRs) including several multi-million-barrel reservoirs in the Middle East region. However, the petroleum industry is quite far behind in its understanding of these reservoir systems, often leading to overly optimistic projections both of the ultimate recovery factor (URF) and of the time span to reach the URF.

In addition to the difficulty to correctly assess the reserves, NFRs also exhibit another difficulty for modeling due to the heterogeneity and immense variations including contrasts in reservoir quality.
In this project, a new methodology for prediction of reservoir quality for field re-development and infill drilling including possible areas of natural fractures was developed. Thereafter, an improved methodology progressing on the latest scientific methods for estimating reserves and matrix oil recovery of NFR reservoirs with a production history was developed. Volumetric properties and phase behavior of the systems was modelled using black oil fluid description. Lastly, a URF method applicable to both NRF fields that already have some production history (brown-fields) and virgin fields (green-fields) was identified. All methods were developed for 3-phase (oil, gas, water) NRF systems.

The contributions have several possible applications in practical petroleum engineering:
Firstly, green-fields can now be evaluated with improved accuracy of URF estimates during development planning.
Secondly, development planning scenarios of well-appraised NFR oil fields can be more accurately evaluated for possible field URF optimization.

Thirdly, decisions regarding installation of longer-term NFR oil facilities as well as predictions for the timing of transition from initial production systems (IPS) to high specification facilities can be made with increased certainty.
Further, NFR oil field URF benchmarks now have an additional cross-reference with the new NFR workflow approach to compare with current industry modelling tools. This may help increase the quality of the URF prediction at all stages of industry practice with an NFR oil field.

Finally, the decision quality for individual well artificial lift system (ALS) selection, correct specifications, and timing has improved for NFR oil fields utilizing the newly provided modelling workflow. The improved workflow should be useful in optimizing individual well operation.



Top depth of the ABC-Field with well locations

Smart Waterflooding in North Sea Chalk

Jiasheng Hao, PhD.

Currently with CNOOC (China)
Full title: "Advanced Waterflooding of North Sea Chalk Reservoirs".
Supervisor: Alexander Shapiro. Co-supervisor: Karen L. Freiberg.
The project was carried out at DHRTC and at CERE.
Funding: DHRTC.

Oil production in the Danish North Sea is at a mature stage. Production often requires a high level of waterflooding. Thus, interest is high in applying advanced – or smart – waterflooding, meaning directed alteration of the content of the different salts (ionic composition) of the injected brine to achieve a better oil recovery. In the project, several possible mechanisms for smart waterflooding were investigated.

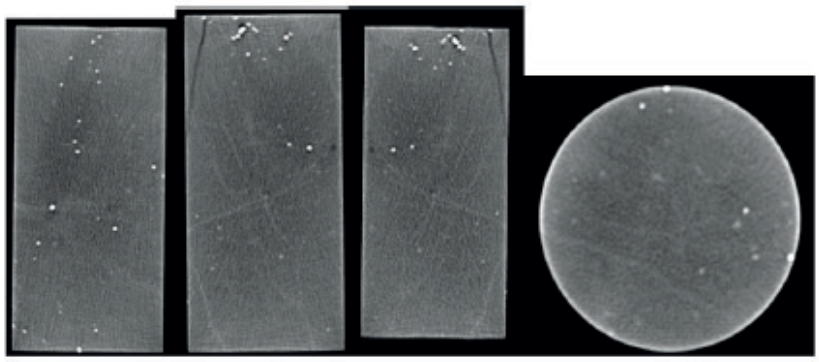
Since the late 1980s, the use of water flooding has become increasingly common for the Danish North Sea fields. It is known from sandstone reservoirs that injection of low salinity brines may result in additional recovery. However, as the carbonate rocks of the North Sea reservoirs are very different from sandstones, low salinity does not always work for them. Instead, a number of other methods have been suggested, including the addition of salts that contain magnesium, calcium, sulfate or other ions. Several possible mechanisms of their action have been discussed such as surface electrostatic interactions, chemical processes, and flow dynamics.

In the project, three aspects of possible recovery mechanisms were investigated: the kinetics of calcite/chalk dissolution and Ca-Mg ion exchange; the effect of flow diversion in sandstone and chalk cores with different levels of heterogeneity; and the impact of chalk compaction on oil recovery during low salinity flooding.
It was found that the dissolution of calcite equilibrates within seconds with low equilibrium concentrations, and that this mechanism is unlikely to cause significant additional production.

As for the Ca-Mg ion exchange on the calcite surface, slow kinetics was seen. Such slow kinetics is unlikely to have a large impact within a laboratory experiment time frame. However, it may be more pronounced on the reservoir scale. For both sandstone and chalk cores, additional recovery was consistently observed from heterogeneous samples. Experiments were accompanied by mathematical simulation. The study demonstrates that core scale heterogeneity is an important factor. Heterogeneity can contribute to recovery through a flow diversion mechanism, which can be triggered by the formation of pore-plugging agents.

In further flooding experiments, the effect of compaction was investigated. It was found that compaction alone was not able to produce large amounts of additional oil. However, compaction combined with heterogeneity could lead to more production. The flow diversion mechanism appeared to be the most plausible explanation.

Overall, the study shows that the time scale (the kinetics) of the chemical processes is important to evaluate their significance under smart waterflooding. Meanwhile, dynamic mechanisms, which take place along with the flow, can play an important role in waterflooding. Recovery from heterogeneous rock samples was consistently higher than from the homogeneous cores. This shows that formation of plugging agents (fines, emulsions, closing the microfractures) and subsequent flow diversion cause a large part of improved oil recovery under smart waterflooding.



A sample X-ray computer tomography scan of a carbonaceous core sample (limestone from the North Sea).

Ionic Liquids for Lithium Batteries

Yingjun Cai, PhD.

Currently with Institute of Process Engineering, Chinese Academy of Sciences.
Full title: "Synthesis and Application of Multifunctional Ionic Liquids for Lithium-Ion Batteries".
Supervisor: Kaj Thomsen. Co-supervisor: Nicolas von Solms.
The project was supported by DTU Chemical Engineering, China Scholarship Council, and the Institute of Process Engineering, Chinese Academy of Sciences.

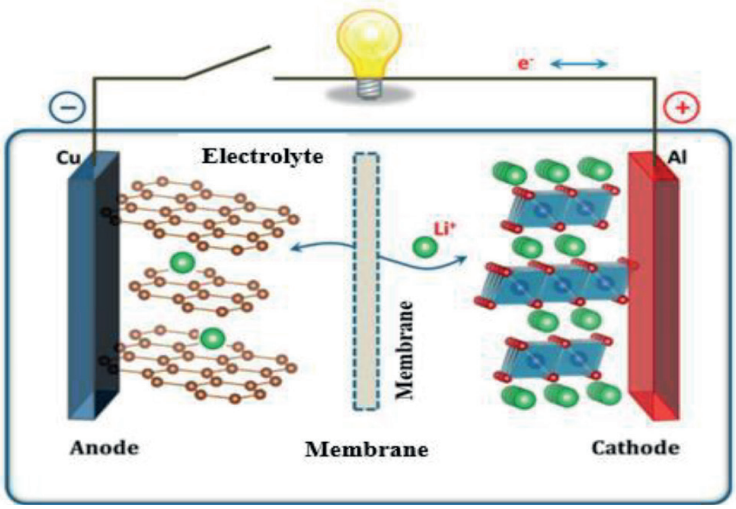
Lithium-ion batteries (LIBs) are currently regarded as the leading battery type for several portable applications. For instance, further improvement of this battery type may contribute to the success of electric vehicles by increasing energy-efficiency and prolonging battery life. In the project, two new types of ionic liquids (ILs) have been developed. Both are shown promising for LIB applications.

Over the recent decade, the lithium-ion battery market has risen sharply, reaching about 50 billion USD in 2020. Compared with other energy storage devices, LIBs have higher energy and power density, higher operating voltage, and longer life cycles.

A key component in LIBs are electrolytes, which affect specific energy density, electrochemical stability, thermo-stability, and properties relating to safety and transport. As new materials are entering the LIB production, new electrolytes will also need to be found. In the project, two new types of ionic liquids (ILs) were synthesized. ILs are organic molten salts containing solely ions. Melting points are below 100 °C. Importantly, ILs can be designed to contain functional groups in anions and cations.

Using two-step methods, 3-(2-amino-2-oxoethyl)-1-vinylimidazolium bis(trifluoromethylsulfonyl) amide ([VAIM][TFSI]) and 1-vinyl-3-propionamide imidazolium bis(trifluoromethylsulfonyl) imide ([VPIM][TFSI]) were synthesized.
The purities of both ILs were determined to be more than 99 %, and their thermal stabilities were high with a range of [VAIM][TFSI] from -30 ± 5 °C to 300 °C, and [VPIM][TFSI] from -50 ± 5 °C to 200 °C.
Both ILs have two functional groups. The basic group can control the water at a low level in LIB-relevant electrolytes, while the unsaturated group can be decomposed at the electrode surface to form a protecting film to improve the capacity, recycling, and rate performance of LIBs.

Three types of electrolytes were applied in different LIB cells, and good results were seen in relation to improved current rate performance and protection against battery breakdown.
In summary, ILs were shown promising as solvents or as additives in electrolytes. The addition of ILs can resolve or reduce safety problems due to their advantages of non-flammability, non-volatility, thermo-stability, and electrochemical stability. Hopefully, the new electrolytes containing ILs will find use in LIBs to enhance their cycling, rate and safety performances.



Structure of lithium ion batteries

Phase Behavior of Inhomogeneous Fluids

Edgar Luis Camacho Vergara, PhD.

Currently process engineer Novo Nordisk
Full title: "Phase Behavior of Inhomogeneous Fluids: A Classical Density Functional Theory Approach".
Supervisor: Xiaodong Liang. Co-supervisor: Georgios M. Kontogeorgis.
Funding: DTU Chemical and Biochemical Engineering.

As inhomogeneous fluids occur in numerous both natural and industrial processes, studying them is of great importance. However, their complexity makes the task challenging. In this PhD project, a novel tool for describing the phase behavior of inhomogeneous fluids has been developed. Importantly, this tool strikes an adequate balance between accuracy and simplicity, making it fit for practical applications in both industry and academia. Such applications involve the calculation of gas adsorption in porous materials, determination of pore size distribution and phase behavior in confined media, and the calculation of the vapor-liquid interfacial tension.

Inhomogeneous fluids comprise physical systems in which fluids are present near an interface (fluid-fluid) or surface (solid-fluid). Characterization of these systems include the determination of several thermodynamic properties such as interfacial tension, adsorption of gases in porous media, capillary condensation and evaporation, and colloid stability. One clear example is the water-air interface. Due to the molecular interactions of water, especially the formation of hydrogen bonds, the interfacial tension of the water-air interface is exceptionally large.

Several approaches have been applied to the study of inhomogeneous systems. Currently, molecular simulations and classical density functional theory (DFT) respectively can be regarded as the most successful methods. Molecular simulations offer a large degree of detail. However, they require a great amount of computational time, making them inaccessible for some practical applications. Therefore, classical DFT has proven to be a successful framework as it combines statistical mechanics concepts used by molecular simulations, together with statistical equations of state that only require a fraction of the computational time required by simulations.

Using thermodynamic perturbation theory with the hard sphere fluid as reference, a classical DFT implementation based on the PC-SAFT equation of state is developed and a thorough comparison with molecular simulations of the individual effects of each of the contributing terms was carried out. Excellent agreement between the two methods was found.
In addition, a new version of the association functional based on thermodynamic perturbation theory (as defined by the PC-SAFT equation of state) and the weighted density approximation is proposed. In comparison to other association functionals, this new approach was shown to provide an adequate balance between simplicity of implementation, CPU time required, and accuracy in the study of confined associated fluids.

A part of the project was devoted to the determination of interfacial tension of vapor-liquid interfaces with classical DFT and the PC-SAFT equation of state. Here, association contributions were taken into account for the calculation of the interfacial tension of substances that are able to form hydrogen bonds, such as alkanols, acetic acid and water. As deviations between classical DFT and experimental data were found, new pure molecular parameters for PC-SAFT were proposed by including the interfacial tension during the fitting procedure. The new parameters were assessed by comparing their performance in the correlation of vapor pressure, liquid density, and interfacial tension for each of the association functionals.

Depiction of interfacial forces at the water-air interface showing a 'water strider' insect floating on the surface.

Overall, the study demonstrates the potential of implementing classical DFT with PC-SAFT to improve our understanding of inhomogeneous fluids.

Bio-fuel Production from Non-food feedstock

Mauro Torli, PhD.

Currently: Postdoc at CERE.
Full title: "Thermodynamics, Design, Simulation and Benchmarking of Bio-fuel Processes".
Supervisors: Philip L. Fosbøl. Co-supervisor: Georgios M. Kontogeorgis.
Funding: DTU and Innovation Fund Denmark. The work is a part of the SYNFERON project.

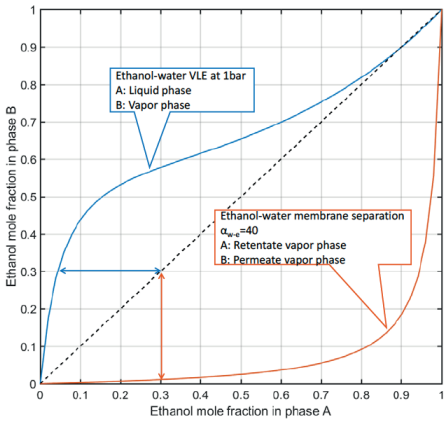
Conversion of lignocellulosic (wood-based) feedstock into fuels has attracted considerable attention. A relatively new approach is production of ethanol from fermentation of CO, CO_2, and H_2O – this mixture is known as syngas. In the project, thermodynamic modeling of processes relevant to this conversion was carried out in support of practical implementation.

Bioethanol makes up the largest share of biofuel production worldwide. However, production is mainly from corn and sugar cane. As these feedstocks are also fit for human and animal consumption, it is highly desirable to produce bioethanol from non-food feedstock instead.

It is possible to produce bioethanol from direct fermentation of lignocellulosic biomass such as dedicated energy crops or agricultural and wood residues etc. However, an alternative bioconversion method has emerged; namely gasifying the feedstock into syngas, which is then fermented. The major benefit is that this process uses all biomass components which can lead to higher conversion factors. Besides lignocellulosic biomass, also municipal solid waste, coal, and natural gas can be gasified and converted into liquid fuels.

With present technology, this route produces aqueous solutions with relatively modest ethanol concentrations, typically below 5 wt%. Hence, it is imperative for economic feasibility that downstream recovery processes are optimized. To that end, accurate thermodynamic modelling is required.

In the project, a y - ϕ phase equilibrium model for description of the phase behavior of 14 gas-solvent systems of relevance is presented. The UNIQUAC model has been selected to calculate the activity coefficients, while the Peng-Robinson EoS or, for systems containing acetic acid, the Hayden-O'Connell Virial EoS were used to calculate the vapor phase fugacities. Further, a method to estimate gas solubility in mixed solvents based on the thermodynamic relation of the Henry's law constant with activity coefficient at finite dilution and the hypothetical liquid standard state fugacity, has been derived.
The proposed model was shown to perform very well even at higher temperatures and pressures. The results show that the UNIQUAC equation, coupled with an appropriate EoS, is able to represent the binaries in the range of temperatures and pressures from 0 to 310 °C and from 1 to 400 bar.
Moreover, various designs for the recovery section of the syngas-to-ethanol process have been benchmarked. The study shows that advance layouts allow for recovery of ethanol from solutions containing less than 4 wt% with operating costs typical of the conventional distillation when applied to aqueous solutions containing 10 wt% alcohol. Mechanical vapor recompression (VRC) presents important improvements compared to the conventional method. The main advantage is the ease of retrofitting; this has already been confirmed by industry experience.
The internally heat-integrated distillation columns and the condenser-reboiler thermal coupling implementation display the highest energy savings. The largest benefits offered by these designs are observed for the lowest ethanol feed concentrations.



Pervaporation selectivity and distillation selectivity for the separation of ethanol from water.

Phase Behavior in High Pressure Oil Recovery

Yiqun Liu, PhD.

Currently postdoc at CERE.
Full title: "High Pressure Phase Behavior of Asymmetric Mixtures for Oil Production".
Supervisor: Wei Yan. Co-supervisors: Teresa Regueira Muniz, Erling H. Stenby.

Until global energy systems have transitioned fully into renewables, production of oil and gas will still be necessary. In recent years, interest in developing deep HPHT (High Pressure High Temperature) reservoirs has risen. These reservoirs often contain volatile oils and gas condensates that are difficult to describe, making development challenging. In the project, HPHT density and phase equilibrium data were measured and utilized for improving thermodynamic models for HPHT reservoir fluids.

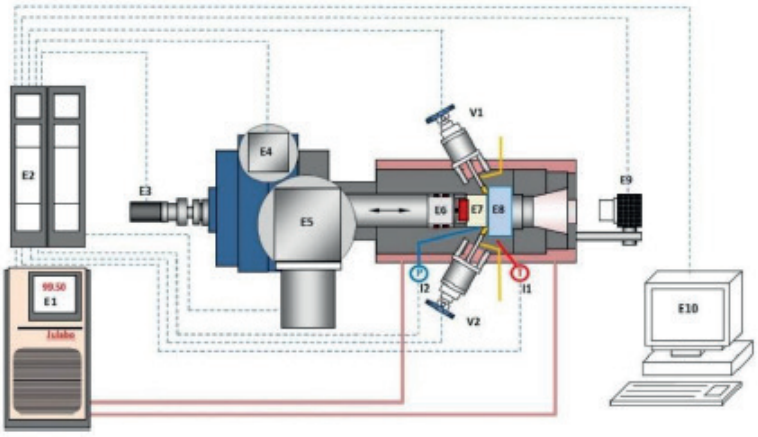
Petroleum reservoirs with temperature higher than 150 °C and pressure higher than 69 MPa are generally referred to as HPHT reservoirs. Examples of HPHT reservoirs under development or exploration can be found in the North Sea, the Gulf of Mexico, and offshore Brazil.

Development of a petroleum reservoir requires an accurate description of the fluid phase behavior in order to determine the reservoir fluid type, estimate the gas and oil in-place, and simulate the production process. Here, description of the density and phase equilibrium of highly asymmetric mixtures is especially relevant for HPHT reservoirs. In the project, live fluid systems were created by combining a light gas component, including carbon dioxide, nitrogen, and methane, and stock tank oil.

The obtained asymmetric multicomponent mixtures are better than well-defined mixtures for mimicking real live fluid samples, which are difficult to obtain from HPHT reservoirs. Their density and phase equilibrium data were systematically measured at temperatures from 298.15 to 463.15 K and pressures up to 1,400 bar. Phase envelopes, relative volumes, and liquid volume fractions below the saturation point were determined.

The data were modeled by three equations of state – Soave-Redlich-Kwong (SRK), Peng-Robinson (PR), and Perturbed Chain Statistical Associating Fluid Theory (PC-SAFT). The performance of the models in saturation pressure proved to be case dependent – no model performed consistently better.

The project also included an experimental and modeling study on systems containing methane/natural gas and mono-ethylene glycol (MEG)/water. The study was carried out at the Equinor research center, Norway. The systems investigated are of direct relevance to tackle gas hydrate issues in subsea pipelines.



The schematic diagram for the PVT 240/1500 visibility cell setup.

Summing up, the measurements in the project have produced valuable HPHT data for evaluating and further improving thermodynamic models for HPHT fluids, thus supporting relevant industrial applications on exploring and developing high-pressure reservoirs. The obtained data can also be used for relevant gas injection modeling.

Plastic from second-generation bio-feedstock

Anne Burniol-Figols, PhD.

Currently with River Stone Biotech.

Full title: "Strategies for Production and Purification of Polyhydroxyalkanoates using Mixed Microbial Consortia – Study on Fermented Crude Glycerol as a Substrate".
Supervisor: Hariklia N. Gavala, co-supervisors: Ioannis Skiadas, Anders E. Daugaard.

Bio-based, biodegradable plastics are desirable as they promise to contribute to less plastic pollution and CO2 emissions than fossil-based plastics do. One group of bio-based plastic of interest is polyhydroxyalkanoates (PHA) due to their high versatility and biodegradability. However, production costs remain too high for PHA to be fully commercially competitive. In the project, strategies for economical production of PHA from second-generation (waste/by-product) bio-feedstock were investigated.

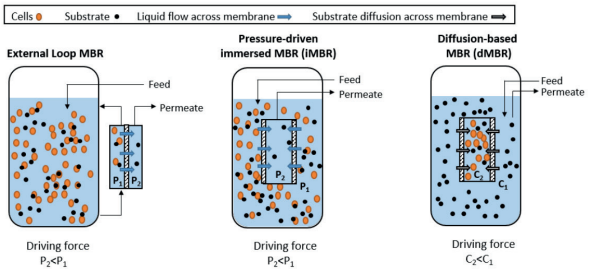
PHA are a group of natural polyesters synthesized as storage polymers in prokaryotic microorganisms. Current commercial production is based on first-generation feedstocks and is associated with high production costs and limited sustainability benefits over conventional fossil-based plastics. Instead, the project seeks to use second-generation byproducts as feedstock; namely crude glycerol which is by-product from the biodiesel industry. Further, the project investigated production based on mixed microbial consortia (MMC). As MMC do not require sterile conditions they contribute in lowering the production cost.

Crude glycerol can be directly converted to PHA by MMC. Prior to production fermentation of the crude glycerol was performed, yielding two products – volatile fatty acids (VFA) and 1,3-propanediol (1,3-PDO) which can be further converted to PHA. Before this project, 1,3-PDO had not been converted into PHA by MMC. However, the obtained PHA yields were low (0.24 Cmol PHA/Cmol 1,3-PDO), and the overall PHA yield was in the same range as direct conversion of crude glycerol to PHA (0.36-0.51 Cmol PHA/Cmol glycerol).

Subsequently, another approach was applied where only VFA was transformed to PHA, while 1,3-PDO was recovered as an additional high-value product. This led to much higher PHA yields from the VFA fraction (up to 0.99 Cmol PHA/Cmol VFA). Compared to a direct conversion of crude glycerol to PHA, this strategy resulted in a higher overall carbon recovery to valuable products (0.73 Cmol/Cmol glycerol).

Thus, this combined process to 1,3-PDO and PHA could be considered as an alternative to the conversion of glycerol to only PHA. The productivity (0.41 g PHA/L/h) was already high in fed-batch mode, but it has the potential to increase even more (up to 1.2 g PHA/L/h) with the use of membrane bioreactors developed in the project.
Besides the study of fermented crude glycerol as a substrate, the project also aimed at developing strategies to improve PHA production and purification beyond this substrate and MMC applied.

Thus, several additional techniques related to PHA production and purification were investigated. Ammonia-based digestion at elevated temperatures allowed for high PHA purity and recovery. The method can be optimized further and most importantly impurities remaining after NH3 digestion did not compromise thermal stability of the polymer. So Combined with the possibility of recycling NH3 in the process the developed method holds high potential for PHA purification.



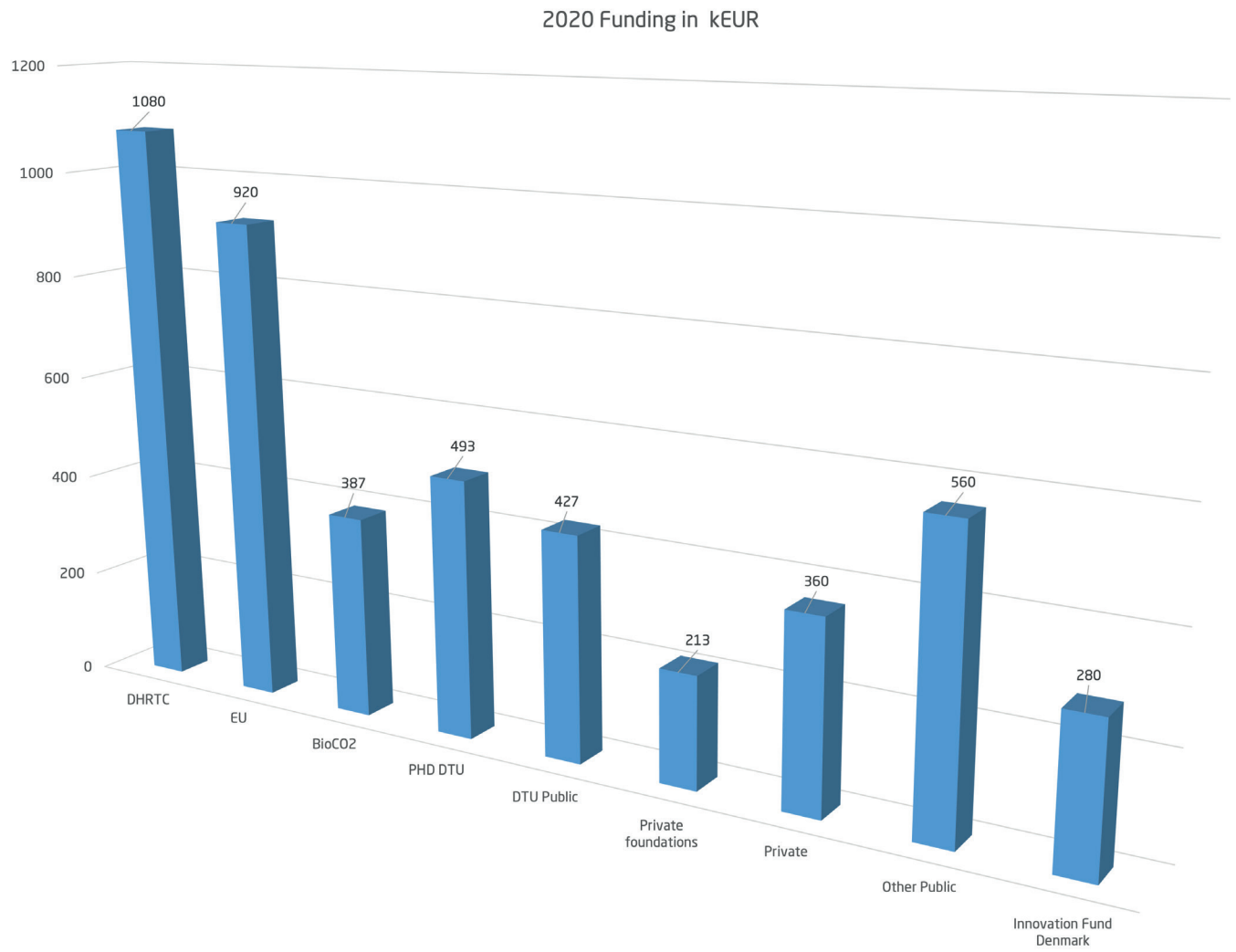
Schematic representation of different MBR configurations. Alternative reactor designs are possible for each configuration. Reproduced from manuscript V and adapted from (Mahboubi et al., 2016).

Funding

As a university research center our objective is to spend all of our money on research. All funding received is 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 2020 fell under the following projects and categories (all amounts in kEUR):



Staff

Faculty

John Bagterp Jørgensen, DTU Compute
Arne Døssing Andreasen, DTU Space
Allan P. Engsig-Karup, DTU Compute
Ida Lykke Fabricius, DTU Civil Engineering
Philip L. Fosbøl, DTU Chemical Engineering
Hariklia Gavala, DTU Chemical Engineering
Georgios M. Kontogeorgis, DTU Chemical Engineering
Xiaodong Liang, DTU Chemical Engineering
Michael L. Michelsen, DTU Chemical Engineering
Thomas G. Petersen, DTU Civil Engineering
Alexander A. Shapiro, DTU Chemical Engineering
Nicolas von Solms, DTU Chemical Engineering
Erling H. Stenby, DTU Chemistry
Kaj Thomsen, DTU Chemical Engineering, Emeritus siden 1.7.2020
Wei Yan, DTU Chemistry

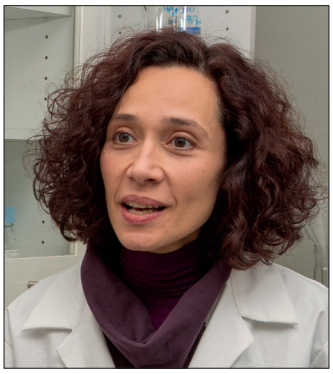
Associated Faculty

Klaus Mosegaard, Niels Bohr Institute

Nicolas von Solms

John Bagterp Jørgensen

Ida Lykke Fabricius



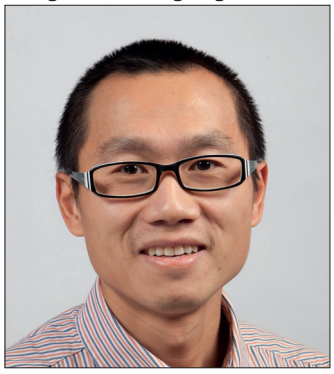
Hariklia Gavala

Georgios M. Kontogeorgis

Erling H. Stenby

Alexander Shapiro

Arne Døssing Andreasen



Xiaodong Liang

Wei Yan

Thomas Guldberg Pedersen

Philip Loldrup Fosbøl

Allan P. Ensig-Karup

Scientific Staff

Antonio Alemany, DTU Chemical Engineering
Susana Almeida, DTU Chemical Engineering
Michael Bache, DTU Chemical Engineering
Nikolaj Blom, DTU Chemical Engineering
Jing Cai, DTU Chemical Engineering
Yuan Chen, DTU Chemical Engineering
Christina Etler, DTU Chemical Engineering
Andrew Holster, DTU Chemical Engineering
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Yang Lei, DTU Chemistry
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Leonardo Meireles, DTU Civil Engineering
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Zahra Nickmand, DTU Chemical Engineering
Martin Due Olsen, DTU Chemical Engineering
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Tian Wang, DTU Chemical Engineering
Rebecka M.L. Werchmeister, DTU Chemistry
Fufang Yang, DTU Chemical Engineering
Yi Yang, DTU Chemistry

Technical and Administrative Staff

Povl Valdemar Andersen, DTU Chemical Engineering
Anne Louise Biede, DTU Chemical Engineering
Christian Ove Carlsson, DTU Chemical Engineering
Thoung Dang, DTU Chemical Engineering
Morten Leth Hjuler, DTU Civil Engineering
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Ditte Jul Valentin, DTU Civil Engineering
Maria del Pilar C. Vidal, DTU Civil Engineering
Duc Thuong Vu, DTU Chemical Engineering
Patricia Wagner, DTU Chemical Engineering
Guoliang Wang, software manager, DTU Chemical Engineering

PhD Students

Wael Almasri, DTU Chemical Engineering
Hadise Baghoee, DTU Chemical Engineering
Martin Malthe Borch, DTU Chemical Engineering
Sebastian Borgquist, DTU Chemical Engineering
Justin Brand, DTU Chemical Engineering
Yingjun Cai, DTU Chemical Engineering
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Yibo Yang, DTU Chemistry

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Yuqiu Chen, DTU Chemical Engineering
Jiasheng Hao, DHRTC
Amirali Rezazadeh, DTU Chemical Engineering
Mirhossein Taheriogtaghsara, DHRTC
Jingrong Zhong, DTU Chemistry

Guests

Henrik Bohr, DTU Chemical Engineering
Rohit Vilas Gaikvad, DTU Chemical Engineering
Yang Lei, DTU Chemistry
Chenyang Zhu, DTU Chemical Engineering

Student Workers

Syed Anas Alam, DTU Chemical Engineering
Caroline Grunnet Rudbeck, DTU Chemical Engineering
Simon Hjort Munk, DTU Chemical Engineering
Jakub Srna, DTU Chemical Engineering

Publications

Published in 2020/2021

CERE 1729
"Antifreeze proteins and gas hydrate inhibition"
Nicolas von Solms
(Antifreeze Proteins and Gas Hydrate Inhibition. In: Ramløv H., Friis D. (eds) Antifreeze Proteins Volume 2. Springer, Cham. (2020))

CERE 1759
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(Geophysics, 85(1) (2020) MR37-MR50; 10.1190/GEO2018-0724.1)

CERE 1878
"Enrichment of mesophilic and thermophilic mixed microbial consortia for syngas biomethanation: the role of kinetic and thermodynamic competition"
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"Density, compressibility and phase equilibrium of high pressure-high temperature reservoir fluids up to 473 K and 140 MPa"
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"Cost optimization and flexibility analysis for the liquefaction of an associated natural gas stream"
Saeed Eini, Georgios M. Kontogeorgis, and Davood Rashtchian
(Journal of Energy Resources Technology, 142 (2020) 062801-1-)

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"Supplementary Material – Cost optimization and flexibility analysis for the liquefaction of an associated natural gas stream"
Saeed Eini, Georgios M. Kontogeorgis, and Davood Rashtchian
(Journal of Energy Resources Technology, 142 (2020) 062801-1-)

CERE 1941
"A review of computer-aided design of paints and coatings"
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(Current Opinion in Chemical Engineering, 27 (2020) 107-120)

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"Comparison of two types of crossover Soave-Redlich-Kwong equations of state for derivative properties of n-alkanes"
Andre P.C.M. Vinhal, Asma Jamali, Hassan Behnejad, Wei Yan, and Georgios M. Kontogeorgis
(Industrial and Engineering Chemistry Research, 59 (2020) 9265-9278)

CERE 1946
"A new study of associating inhomogeneous fluids with classical density functional theory"
Edgar L. Camacho Vergara, Georgios M. Kontogeorgis, and Xiaodong Liang
(Molecular Physics, 118(9-19) (2020) e1725668-; DOI: 10.1080/00268976.2020.1725668)

CERE 1947

"A multi-layered view of chemical and biochemical engineering"
Rafiqul Gani, Jerzy Baldyga, Béatrice Biscans, Elisabetta brunazzi, Jean-Claude Charpentier, Enrico Drioli, Hermann Feise, Andrew Furlong, Kevin M. Van Geem, Jean-Charles de Hemptinne, Antoon J.B. ten Kate, Georgios M. Kontogeorgis, Flavio Manenti, Guy B. Marin, Seyed Soheil Mansouri, Patrick M. Piccione, Ana Povoa, Manuel Andres Rodrigo, Bent Sarup, Eva Sorensen, Isuru A. Udugama, and John M. Woodley
(Chemical Engineering Research and Design, 155 (2020) 133-145)

CERE 1952

"Polyhydroxyalkanoate (PHA) purification through dilute aqueous ammonia digestion at elevated temperatures"
A. Burniol-Figols, I. V. Skiadas, A. E. Daugaard, and H. N. Gavala
(Journal of Chemical Technology and Biotechnology, 95(5) (2020) 1519-1532)

CERE 1953

"Cryopreservation and fast recovery of enriched syngas-converting microbial communities"
Antonio Grimalt-Alemany, Mateusz Łezyk, Konstantinos Asimakopoulos, Ioannis V. Skiadas, Hariklia N. Gavala
(Water Research, 177 (2020) 115747-; DOI: 10.1016/j.watres.2020.115747)

CERE 1954

"Temperature Effects on Syngas Biomethanation Performed in a Trickle Bed Reactor"
K. Asimakopoulos, M. Łężyk, A. Grimalt-Alemany, A. Melas, Z. Wen, H. N. Gavala, I. V. Skiadas
(Chemical Engineering Journal, 393 (2020) 124739-https://doi.org/10.1016/j.cej.2020.124739)

CERE 2002

"Studies on temperature characteristics and initial formation interface during cyclopentane-methane hydrate formation in large-scale equipment with bubbling"
Jing Cai, Tao Lv, Yu Zhang, Nicolas von Solms, Chun-Gang Xu, Zhao-Yang Chen, and Xiao-Sen Li
(Applied Energy, 258 (2020) 114076-)

CERE 2003

"Process analysis of shea butter solvent fractionation using a generic systematic approach"
Olivia Perederic, Seyed Mansouri, Sten Appel, Bent Sarup, Rafiqul Gani, John Woodley, and Georgios M. Kontogeorgis
(Industrial and Engineering Chemistry Research, 59 (2020) 9265-9278)

CERE 2004

"Screening of amino acids and surfactant as hydrate promoter for CO_2 capture from flue gas"
Jyoti Shanker Pandey, Yousef Jouljamal Daas, and Nicolas von Solms
(Processes, 8 (2020) 124-)

CERE 2005

"Inhibition of natural gas hydrate in the system containing salts and crude oil"
Liang Mu, and Nicolas von Solms
(Journal of Petroleum Science and Engineering, 188 (2020) 106940-)

CERE 2006

"The effect of concentration of lithium salt on the structural and transport properties of ionic liquid-baseed electrolytes"
Jiahuan Tong, Shengli Wu, Nicolas von Solms, Xiaodong Liang, Feng Huo, Qing Zhou, Hongyan He, and Suojiang Zhang
(Frontiers in Chemistry, 7 (2020) 1-)

CERE 2008

"Predicting activity coefficients with the Debye-Hückel theory using concentration dependent static permittivity"
Qun Lei, Baoliang Peng, Li Sun, Jianhui Luo, Yuan Chen, Georgios M. Kontogeorgis, and Xiaodong Liang
(AIChE Journal, 66(11) (2020) E16651-)

CERE 2009

"Thermodynamic Theory of Diffusion and Thermodiffusion Coefficients in Multicomponent Mixtures"
Alexander A. Shapiro
(Jounal of Non-Equilibrium Thermodynamics, 45(4) (2020) 343-372)

CERE 2010

"Coalescence of oil droplets in microchannels under brine flow"
Tian Wang, Simon Ivar Andersen, and Alexander Shapiro
(Colloids and Surfaces A, 598 (2020) 124864-)

CERE 2013

"Density, viscosity, and conductivity of [VAIM][TFSI] in mixtures for lithium-ion battery electrolytes"
Yingjun Cai, Nicolas von Solms, Suojiang Zhang, and Kaj Thomsen
(Journal of Chemical & Engineering Data, 65 (2020) 495-502)

CERE 2015

"Analysis of Some Electrolyte Models Including Their Ability to Predict the Activity Coefficients of Individual Ions"
Li Sun, Xiaodong Liang, Nicolas von Solms, and Georgios M. Kontogeorgis
(Industrial & Engineering Chemistry Research, 59(25) (2020) 11790-11809)

CERE 2017

"Matching the critical point of associating fluids with the Cubic Plus Association equation of state"
Xiaodong Liang, Baoling Peng, Yuan Chen, Jianhui Luo, Michael Locht Michelsen, and Georgios M. Kontogeorgis
(Fluid Phase Equilibria, 526 (2020) 112674-)

CERE 2020

"Coalscence of oil droplets in microchannels under brine flow"
Tian Wang, Simon Ivar Andersen, and Alexander Shapiro
(Colloide and Surfaces A, 598 (2020) 124864-)

CERE 2021

"Group Contribution Method to Estimate the Biodegradability of Organic Compounds"
Spardha Jhamb, Irène Hospital, Xiaodong Liang, Francis Pilloud, Patrick M. Piccione, and Georgios M. Kontogeorgis
(Industrial & Engineering Chemistry Research, 59(47) (2020) 20916-20928)

CERE 2024

"Gas solubility in ionic liquids: UNIFAC-IL model extension"
Yuqiu Chen, Xinyan Liu, John M. Woodley, Georgios M. Kontogeorgis
(Ind. Eng. Chem. Res., 59 (2020) 16805-16821)

CERE 2025

"Methane hydrate formation, storage and dissociation behavior in unconsolidated sediments in the presence of environment-friendly promoters"
Jyoti Shanker Pandey, Yousef Jouljamal Daas, and Nicolas von Solms
(SPE-200532-MS)

CERE 2026

"On the study of the vapor-liquid interface of associating fluids with classical density functional theory"
Edgar L. Camacho Vergara, Georgios M. Kontogeorgis, and Xiaodong Liang
(Fluid Phase Equilibria, 522 (2020) 112744-)

CERE 2027

"An experimental study on improved production performance by depressurization combined with CO2-enriched air injection"
Meng Shi, John M. Woodley, and Nicolas von Solms
(Energy Fuels, 34 (2020) 7329-7339)

CERE 2028

"Porosity in chalk – roles of elastic strain and plastic strain"
I.L. Fabricius
(Sedimentology, 67 (2020) 3451-3470)

CERE 2030

"Multifunctional imidazolium-based ionic liquid as additive for silicon/carbon lithium ion batteries"
Yingjun Cai, Tinghua Xu, Nicolas von Solms, Haitao Zhang, and Kaj Thomsen
(Electrochimica Acta, 340 (2020) 135990-)

CERE 2031

"Solubility modeling of air in aqueous electrolyte solutions with the e-CPA equation of state"
Li Sun, Xiaodong Liang, Nicolas von Solms, and Georgios M. Kontogeorgis
(Industrial & Engineering Chemistry Research, 59(41) (2020) 18693-18704)

CERE 2032

"Heat capacities of fluids: The performance of various equations of state"
Chenyang Zhu, Xiangyang Liu, Maogang He, Georgios M. Kontogeorgis, and Xiaodong Liang
(Journal of Chemical & Engineering Data, 65(12) (2020) 5654-5676)

CERE 2033

"Evaluating the performance of the PC-SAFT and CPA equations of state on water´s anomalous properties"
Evangelos Tsochantaris, Xiaodong Liang, and Georgios M. Kontogeorgis
(Journal of Chemical & Engineering Data, 65(12) (2020) 5718-5734)

CERE 2035

"Effect of N2/H2 injection on CH4 hydrate decomposition"
Jin-Rong Zhong, Yi-Fei Sun, Yan Xie, Chang-Yu Sun, Guang-Jin Chen, and Wei Yan
(Chemical Engineering Journal, 396 (2020) 125266-)

CERE 2038

"Enhanced CH4-CO2 Hydrate Swapping in the Presence of Low Dosage Methanol"
Jyoti Shanker Pandey, Charilaos Karantonidis, Adam Paul Karcz, and Nicolas von Solms
(Energies, 13 (2020) 5238-; doi:10.3390/en13205238)

CERE 2044

"Enhanced Hydrate-Based Geological CO_2 Capture and Sequestration as a Mitigation Strategy to Address Climate Change"
Jyoti Shanker Pandey, Yousef Jouljamal Daas, Adam Paul Karcz, and Nicolas von Solms
(Energies, 13 (2020) 5661-; doi:10.3390/en13215661)

CERE 2046

"Water-flooding and consolidation of reservoir chalk – effect on porosity and Biot's coefficient"
T.B. Gram, F.P. Ditlevsen, K. Mosegaard, and I.L. Fabricius
Geophysical Prospecting, 69 (2021) 495–513)

CERE 2047

"Experimental determination of relative permeabilities and critical gas saturations under solution-gas drive"
Wael Al-Masri, Alexander Shapiro
(Journal of Petroleum Science and Engineering 202 (2021) 108509)

CERE 2048

"A new approach to thermal segregation in petroleum reservoirs: Algorithm and case studies"
Hadise Baghooee, François Montel, Guillaume Galliero, Wei Yan Alexander Shapiro
(Journal of Petroleum Science and Engineering 201 (2021) 108367)

CERE 2049

"Continuous upscaling and averaging"
Alexander A. Shapiro
(Chemical Engineering Science 234 (2021) 116454)

CERE 2050

"Solid-Liquid Equilibria of a 30 wt % Aqueous Monoethanolamine Solution Containing Urea and Monoethylene Glycol"
Randi Neerup, Sebastian Villadsen, Kaj Thomsen, Philip Fosbøl
(J. Chem. Eng. Data, 66 (2021), 222–233)

CERE 2052

"An offshore reservoir monitoring system based on fiber optic sensing of seabed strains",
Eyal Levenberg, Ivanka Orozova-Bekkevold Ivanka
(First Break, 38(3) (2020) 35-41; doi: 10.3997/1365-2397.fb2020016)

CERE 2053

"Numerical Forward Modeling of the Overpressure Build-up in the Cenozoic Section of the Central Graben in the North Sea"
Ivanka Orozova-Bekkevold, and Thomas G. Petersen,
(Accepted for by Petroleum Exploration and Production Technology Manuscript number: PEPT-S-20-00569)

CERE 2055

"Direct Visualization of CH4/CO2 Hydrate Phase Transitions in Sandstone Pores"
Jyoti Shanker Pandey, Ørjan Strand, Nicolas von Solms, Geir Ersland, and Stian Almenningen
(https://doi.org/10.1021/acs.cgd.0c01714)

CERE 2057

"Modeling the thermal conductivity of hydrofluorocarbons, hydrofluoroolefins and their binary mixtures using residual entropy scaling and cubic-plus-association equation of state"
Hangtao Liu, Fufang Yang, Xiaoxian Yang, Zhen Yang, Yuanyuan Duan
(Journal of Molecular Liquids, 330 (2021) 115612-)

CERE 2059

"Improving the Anaerobic Digestion of Swine Manure through an Optimized Ammonia Treatment: Process Performance, Digestate and Techno-Economic Aspects"
A. Lymperatou, N.B. Rasmussen, H.N. Gavala, I.V. Skiadas
(Energies, 14 (2021) 787-)

CERE 2060

"Commodity chemical production from 3rd generation biomass: A techno-economic assessment of lactic acid production"
Elena Tomas Grasa, O. Ögmundarson, N. H. Gavala, and S. Sukumara
(Biofuels Bioproducts & Biorefining, 15 (2021) 257-281); https://doi.org/10.1002/bbb.2160)

CERE 2061

"Biofouling mitigation approaches during water recovery from fermented broth via forward osmosis Membranes"
S. Kalafatakis, A. Zarebska, L. Lange, C. Helix-Nielsen, I. V. Skiadas, and H. N. Gavala
(Membranes, 10 (2020) 307-; doi:10.3390/membranes10110307)

CERE 2062
"Gas biological conversions: the potential of Syngas and Carbon Dioxide as production platforms"
H. N. Gavala, A. Grimalt-Alemany, K. Asimakopoulos, and I. V. Skiadas
(Waste and Biomass Valorization, (2021) https://doi.org/10.1007/s12649-020-01332-7

CERE 2063
"Enhancing polyhydroxyalkanoate productivity with cell-retention membrane bioreactors"
Anna Burniol-Figols, Manuel Pinelo, Ioannis V. Skiadas, Hariklia N. Gavala
(Biochemical Engineering Journal, 161 (2020) 107687-)

CERE 2064
"High-pressure experimental and theoretical study of CO2 solubility in aqueous blends of lysine salts with piperazine as new absorbents"
Suleman, Humbul, Abdulhalim Shah Maulud, Afaf Syalsabila, Muhammad Zubair Shahid, and Philip Loldrup Fosbøl
(Fluid Phase Equilibria, 507 (2020) 112429-)

CERE 2065
"Scalar magnetic difference inversion applied to UAV-based UXO Detection"
Mick Emil Kolster and Arne Døssing Andreasen
(Geophys. J. Int., 224 (2020) 468-486)

CERE Publications, Submitted in 2020, under review

CERE 2001
"Insights into CO_2 capture by flue gas hydrate formation using selected amono acids"
Jyoti Shanker Pandey, Yousef Jouljamal Daas, and Nicolas von Solms
(Replaced by CERE 2044)

CERE 2011
"Kinetics of calcite dissolution and Ca-Mg ion exchange on the surfaces of North Sea chalk powders"
Jiasheng Hao, Karen L. Feilberg, and Alexander Shapiro
(Submitted for publication)

CERE 2012
"Effect of flow diversion on oil recovery under smart waterflooding in homogenous and heterogeneous chalk and sandstone"
Jiasheng Hao, Petro Nakutnyy, and Alexander Shapiro
(Submitted for publication)

CERE 2014
"A model for relative permeabilities under gas liberation or condensate precipitation in porous media"
Wael Al-Masri, and Alexander Shapiro
(Submitted for publication)

CERE 2016
"Good reporting practice for thermo-physical and thermochemical property measurements (IUPAC Technical Raport)
Ala Bazyleva, Jens Abildskov, Andrzej Anderko, Olivier Baudouin, Yury Chernyak, Jean-Charles de Hemptinne, Vladimir Diky, Ralf Dohrn, J. Richard Elliott, Johan Jacquemin, Jean-Noel Jaubert, Kevin G. Joback, Ursula R. Kattner, Georgios M. Kontogeorgis, Herbert Loria, Paul M. Mathias, John P. O´Connell, Wolfram Schröer, G. Jeffrey Smith, Ana Soto, Shu Wang, and Ronald D. Weir
(Submitted for publication)

CERE 2018
"Vibrational spectra and conformations for chiral opioids in changing solvents"
Michael Bache, Karin Stibius, Rolf W. Berg, Nikolaj S. Blom, and Henrik Georg Bohr
(Submitted for publication)

CERE 2022
"State function-based flash specifications for open systems in the absence or presence of chemical reactions"
Fernando de Azevedo Medeiros, Erling H. Stenby, and Wei Yan
(Submitted for publication)

CERE 2023
"Density modeling of high-pressure mixtures using cubic and non-cubic EoS and an excess volume method"
Wei Yan, Teresa Regueira, Yiqun Liu, and Erling H. Stenby
(Submitted for publication)

CERE 2029
"Costa Tsonopoulos - his legacy and some personal reflections on cubic equations of state and beyond"
Ioannis Tsivintzelis, Eirini Karakatsani, and Georgios M. Kontogeorgis
(Submitted for publication)

CERE 2034
"A methodology to predict thermodynamic data from spectroscopic analysis"
Antoon J.B. ten Kate, Jan Gerretzen, Henk-Jan von Manen, Georgios M. Kontogeorgis, and Gerrald Bargeman
(Submitted for publication)

CERE 2037
"Phase Envelope Calculations of Synthetic Gas Systems with a Cros-over Equation of State"
Andre P. C. M. Vinhal, Wei Yan, and Georgios M. Kontogeorgis
(Submitted for publication)

CERE 2039
"Effect of flow diversion on oil recovery under smart waterflooding in homogenous and heterogeneous chalk and sandstone"
Jiasheng Hao, Petro Nakutnyy, and Alexander Shapiro
(Internal report)

CERE 2041
"An open-access database of the thermophysical properties of nanouids"
Maria E. Mondejar, Maria Regidor, Joerg Krafczyk, Christian Ihmels, Bastian Schmid, Georgios M. Kontogeorgis, and Fredrik Haglind
(Submitted for publication)

CERE 2042
"Industrial requirements for thermodynamic and transport properties - 2020"
Georgios M. Kontogeorgis, Ralf Dohrn, Ioannis G. Economou, Jean-Charles de Hemptinne, Antoon ten Kate, Susanna Kuitunen, Miranda Mooijer, Ljudmila Fele Želnik, and Velisa Vesovic
(Submitted for publication)

CERE 2043
"Effects of resonant electromagnet fields on bio-film formation in pseudomonas aeruginosa"
Janus AJ Haagesen, Michael Bache, Livio Giuliani, and Nikolaj Blom
(Submitted for publication)

CERE 2051

"Viscosity of binary refrigerant mixtures of R32 + R1234yf and R32 + R1243zf"

Xiaoxian Yang, Hangtao Liu, Shi Hai Chen, Dongchan Kim, Fufang Yang, Arash Arami-Niya, Yuanyuan Duan
(Submitted for publication)

CERE 2054

"Chemically Modified Hydrate Swapping and Hydrate Stability during Multistage CO2-N2 Injection Schemes"

Jyoti Shanker Pandey, Saad Khan, Adam Paul Karcz & Nicolas von Solms
(Submitted for publication)

CERE 2056

"Influence of Amino Acids on CH4 Gas Hydrate Formation & Dissociation Kinetics Above and Below 0°C"

Jyoti Shanker Pandey, Saad Khan, Wenjun Wang, Nicolas von Solms
(Submitted for publication)

CERE 2058

"Analysis of the thermodynamic performance limits of the organic Rankine cycle in low and medium temperature heat source applications"

Fubin Yang, Fufang Yang, Jian Li, Shuozhuo Hu, Zhen Yang, Yuanyuan Duan
(Submitted for publication)

M.Sc. students, 2020

Jacob Thejl Petersen, "Drone-borne magnetic data from Perros-Guirec, France in relation to mineral exploration", Arne Døssing Andreasen

Ebuka Malachi Eya, "Petrophysical log interpretation in deviated wells", Ida Lykke Fabricius

Ertol Zhurda, "Mechanisms controlling strength development of remolded chalk over time", Ida Lykke Fabricius & Tobias Orlander

Jacobo Resouso Casas, "Simulation and optimization of CO_2 enhanced ethanol stripping", Philip L. Fosbøl

Thor Kell Engelsen, "Biomass composition effects on the efficiency of aqueous ammonia soaking as a method to enhancing the methane potential", Hariklia Gavala

Sotirios Efstathios Antonoudis, "Continuous anaerobic co-digestion of swine manure with pre-treated and raw carbon-rich biomasses", Hariklia Gavala

Carlos Alfonso González López de Lerma, "Processing of seaweed for biological production of bulk chemicals", Hariklia Gavala

Mohammad Balkiss, "Recovery of ammonia from aqueous ammonia soaked biomass", Hariklia Gavala

Pedro Velho Ferreira, "Development of a predictive thermodynamic model based on the CPA equation of state", Georgios M. Kontogeorgis and and Xiaodong Liang

Richard Kendal, "Analysis of wellbore stability and drilling practices in deep onshore wells in Denmark with respect to future geothermal installations. Zone I - North Jylland", Ivanka Orozova-Bekkevold

Periklis Isaakidis, "Analysis of wellbore stability and drilling practices in deep onshore wells in Denmark with respect to future geothermal installations. Zone II - Sealand, Fyn and South Jylland", Ivanka Orozova-Bekkevold

Evgenia Chatzivasileiou, "Free swell of clay and links to mineralogy", Thomas G. Petersen

Xabier Yarzabal Barandika, "Can drill cuttings be used to predict clay swelling behavior?", Thomas G. Petersen

Anders Jens Bloch, "Drone-baseret geofysisk kortlægning af tungsandsmineraler", Thomas G. Petersen & Arne Døssing Andreasen

Clement C.G. Daguet, "Changes of fuel oxidation", Erling H. Stenby

Sebastian Borgquist, "CO_2 Capture by absorption - vapor-liquid equilibrium measurement and modeling", Kaj Thomsen

Charilaos Karantonidis, "Methane production and CO_2 storage in a porous medium with promotor", Nicolas von Solms

Saad Khan, "Multistage CH_4-CO_2 swapping in porous medium", Nicolas von Solms

Conference contributions & Invited speakers

JANUARY

The Impact Conference Davos Blockbase, Schweiz, 20-26 January 2020

Nikolaj Sorgenfrei Blom, "What if water is the technology we have been waiting for?", The Impact Conference Davos Blockbase, Schweiz, 20-26 January 2020 (Invited speaker)

FEBRUARY

9th Mini symposium on Poroelasticity, University of Lausanne, Lausanne, Switzerland, 11. February 2020

Leonardo Meireles, Chuangxin Lyu, Thomas Ingeman-Nielsen,
"Impact of sub-zero temperature changes on P and S-wave velocities in a permafrost sample undergoing cyclical loading", 9th Mini symposium on Poroelasticity, University of Lausanne, Lausanne, Switzerland, 11. February 2020 (Oral)

Leonardo Meireles, Ida Lykke Fabricius, "Softening and weakening of soft and stiff outcrop chalk prompted by changes in pore water composition", 9th Mini symposium on Poroelasticity, University of Lausanne, Lausanne, Switzerland, 11. February 2020 (Poster)

Gordon Research Seminar on Natural Gas Hydrate Systems, Galveston, United States 22-23 February 2020

J. S. Pandey, S. Almenningen, N. von Solms, G. Ersland, "Visualization of CH4 Hydrate Dissociation Under Permafrost Temperature Conditions Using High-Pressure Micromodel", Gordon Research Seminar on Natural Gas Hydrate Systems, Galveston, United States 22-23 February 2020 (Oral)

Gordon Research Conference on Natural Gas Hydrate Systems, Galveston, United States, 23-28 February 2020

J. S. Pandey, Ø. Strand, N. von Solms, S. Almenningen, G. Ersland, "Direct Visualization of CH4/CO2 Mixed Hydrate Phase Transitions in Porous Media", Gordon Research Conference on Natural Gas Hydrate Systems, Galveston, United States, 23-28 February 2020 (Poster)

MARCH

DAREDISRUPT Fireside chat for HAFSLUND Energy, Norway, 2 March 2020

Nikolaj Sorgenfrei Blom, "What if water is the technology we have been waiting for?", DAREDISRUPT Fireside chat for HAFSLUND Energy, Norway, 2 March 2020 (Invited speaker)

MAY

EGU2020-13678 May 5 2020 EGU 2020 General Assembly Online

H.D. Holmslykke, C. Kjøller, R. Weibel, I.L. Fabricius "Laboratory and modelling investigations of potential geochemical reactions upon seasonal heat storage in Danish geothermal reservoirs" EGU2020-13678 May 5 2020 EGU 2020 General Assembly Online (Oral)

Virtual DHRTC Young Researchers Day, Kgs. Lyngby, Denmark, 15 May 2020

Sindhu Vudayagiri, Zahra Nickmand, Johannes Liljenhjerte, Jens Vinge Nygaard, Nicolas von Solms, "Extended Coiled Tubing Reach", Virtual DHRTC Young Researchers Day, Kgs. Lyngby, Denmark, 15 May 2020 (Poster)

Zahra Nickmand, Johannes Liljenhjerte, Sindhu Vudayagiri, Nicolas von Solms, Jens Vinge Nygaard, "Extended Coiled Tubing Reach", Virtual DHRTC Young Researcher's Day, Kgs. Lyngby, Denmark 15 May 2020 (Oral)

JUNE

ATOMS virtual seminar, Brazil, 4 June 2020

Fernando Medeiros, "State Function-Based Flash Specifications for Open Systems - Application to CO2 Underground Geological Storage", ATOMS virtual seminar, Brazil, 4 June 2020 (Oral)

AUGUST

World of Wisdom transdisciplinary conference,Visby, Gotland, Sweden, 11-16 August 2020

Nikolaj Sorgenfrei Blom, "Water Bridging theme", World of Wisdom transdisciplinary conference,Visby, Gotland, Sweden, 11-16 August 2020 (Co-hosting sessions with Prof. Anders Nilsson and Prof. Gerald Pollack)

ATOMS virtual seminar, Brazil, 13 August 2020

Georgios M. Kontogeorgis, "The legacy of the Debye-Huckel equation for electrolyte solutions. 100 years of stories, facts, myths, and lies - how should we proceed?", ATOMS virtual seminar, Brazil, 13 August 2020 (Oral)

Virtual ESCAPE 30, The 30th European Symposium on Computer Aided Process Engineering Milan, Italy, 30 August-2 September 2020

O. A. Perederic, A. Mountraki, E. Papadopoulou, J. M. Woodley, G. M. Kontogeorgis, "Life Cycle Analysis of Phenol - Formaldehyde Resins Substituted with Lignin", Virtual ESCAPE 30, The 30th European Symposium on Computer Aided Process Engineering Milan, Italy, 30 August-2 September 2020 (Poster)

Interpore 2020 Online conference, Brussels, Belgium, 31 August-4 September

Al-Masri, W., Shapiro, A.A., "The Effect of Solution Gas Liberation on Oil Flow in Porous Media", Interpore 2020 Online conference, Brussels, Belgium, 31 August-4 September 2020 (Oral)

J. S. Pandey, N. von Solms, "Flue Gas Hydrate Storage, Self-Preservation and Dissociation in Unconsolidated Porous Medium in the Presence of Environment-Friendly Promoters", Interpore 2020 Online conference, Brussels, Belgium, 31 August-4 September 2020 (Oral)

J. S. Pandey, S. Almenningen, N. von Solms, G. Ersland, "Visualization of CH4 Hydrate Dissociation Under Permafrost Temperature Conditions Using High-Pressure Micromodel", Interpore 2020 Online conference, Brussels, Belgium, 31 August-4 September 2020 (Oral)

SEPTEMBER

ECMOR, United Kingdom, 14-17 September 2020

Fernando Medeiros, "Modified RAND Algorithms for Multiphase Geochemical Reactions", ECMOR virtual conference, United Kingdom, 14-17 September 2020 (Poster)

NOVEMBER

Online conference "Modelling & Simulation in Formulations", Royal Society of Chemistry, London, UK, 10 November 2020

Georgios M. Kontogeorgis, Spardha Jhamb, Xiaodong Liang, and Kim Dam-Johansen, "Computer-Aided Design of Paints and Coatings - A revies and recent applications", Online conference "Modelling & Simulation in Formulations", Royal Society of Chemistry, London, UK, 10 November 2020 (Oral)

2020 Virtual AIChE Annual Meeting, 15-20 November 2020

R. Neerup, I. A. Løge, D. C. Figueroa Murcia, K. Thomsen, P. L. Fosbøl, "Thermodynamic Modelling of FeCO3 Solubility Using the Extended Uniquac Model", 2020 Virtual AIChE Annual Meeting, 15-20 November 2020 (Oral)

2nd International Workshop (online) on Numerical and experimental modelling of wave structure interactions, 17-26 November, 2020

A.P. Engsig-Karup, "High-Order Numerical Methods for Nonlinear Wave and Wave-Structure Interaction for Engineering Applications", 2nd International Workshop (online) on Numerical and experimental modelling of wave structure interactions, 17-26 November, 2020 (Invited plenary talk)

DHRTC Webinar: Well Technology, November 20, 2020

Sindhu Vudayagiri, Zahra Nickmand and Nicolas von Solms, "Extended Coiled Tubing Reach: ES Material", DHRTC Webinar: Well Technology, November 20, 2020 (Oral presentation).

Zahra Nickmand and Nicolas von Solms, "Extended Coiled Tubing Reach: Design and Make Experimental Set up", DHRTC Webinar: Well Technology, November 20, 2020 (Oral)

DECEMBER

2020 AGU Fall Meeting - Online event, Washington, United States, 1-7 December 2020

J. S. Pandey, C. Karantonidis, A. P. Karcz, N. von Solms, "Low Dosage Chemical Assisted Enhanced CH4 Production and CO2 Storage in Porous Medium During Hydrate Swapping", 2020 AGU Fall Meeting - Online event, Washington, United States, 1-7 December 2020 (Poster)

SPE Europec featured at 82nd EAGE Conference and Exhibition, Amsterdam, Netherlands, 8-11 December 2020

J. S. Pandey, Y. J. Daas, N. von Solms, "Methane Hydrate Formation, Storage and Dissociation Behavior in Unconsolidated Sediments in the Presence of Environment-friendly Promoters", SPE Europec featured at 82nd EAGE Conference and Exhibition, Amsterdam, Netherlands, 8-11 December 2020 (Oral)

Online conference EAGE Near Surface Geoscience 2020 (NSG2020), Brittany, France, 7-8 December 2020

Arne Døssing Andreasen, G. Martelet, T.M.Rasmussen, E.da Silva, "A Multidisciplinary UAV- and Ground-Geophysical Mapping of Complex Mineralisations in an Inter-Tidal Coastal Zone", Online conference EAGE Near Surface Geoscience 2020 (NSG2020), Brittany, France, 7-8 December 2020 (Oral)

Mark D. Wigh, T. M. Hansen, Arne Døssing Andreasen, "Probabilistic Inversion of Magnetic UXO Data: Implementing Prior UXO Data from the North Sea", Online conference EAGE Near Surface Geoscience 2020 (NSG2020), Brittany, France, 7-8 December 2020 (Oral)

Jirigalatu Jirigalatu, A. Døssing, "Noise Analysis of a Portable Aeromagnetic Surveying System Using a Hybrid UAV", Online conference EAGE Near Surface Geoscience 2020 (NSG2020), Brittany, France, 7-8 December 2020 (Poster)