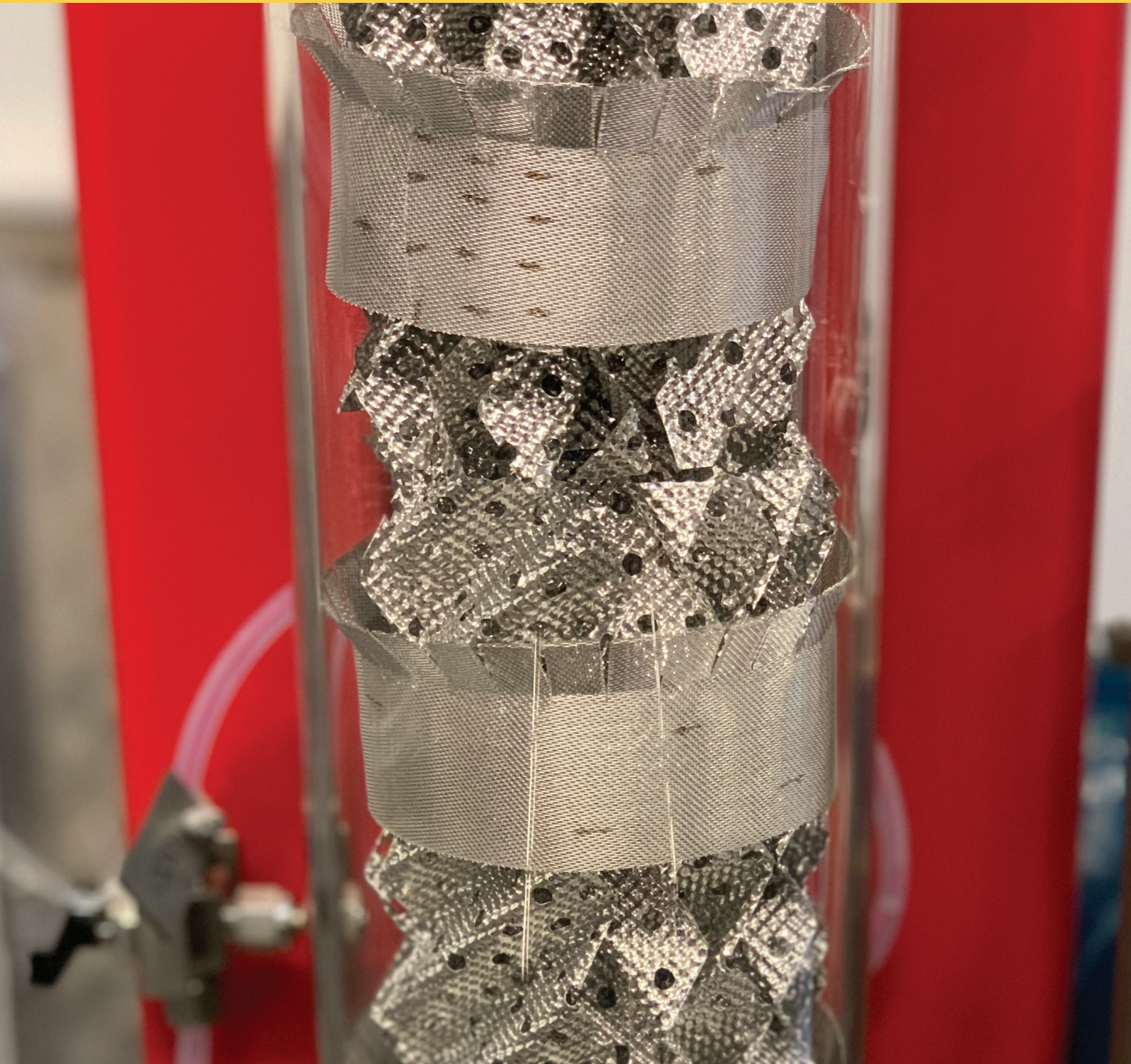
DTU

Center for Energy Resources Engineering

CERE
Annual Report 2019



CERE Annual Report 2019

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

Phone: +45 45 25 20 12
Fax: +45 45 88 22 58

Website:
www.cere.dtu.dk

Editor-in-chief:
Georgios Kontogeorgis, 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

"The cover photo shows a section of DTU's 10 m high pilot-scale packed-column absorber for studying carbon capture in realistic scenarios. Such demonstration-scale equipment (i.e. beyond laboratory) for carbon capture will play an increasingly important role as we attempt to solve the problem of man-made greenhouse gas emissions"

Contents

Introduction 4

Industry Consortium 5

Carbon Capture 10

Electrolytes 12

Oil And Gas Applications 16

Algorithms 20

Water Research 22

News From Cere 24

Synergy With Kt-Consortium 29

Phd 34

Staff 41

Publications 43

Conference Contributions & Invited Speakers, 2019 46

INTRODUCTION

10 Years of CERE

In 2009, Center for Energy Resources Engineering was established as an interdepartmental center at DTU. With its core being the chemical engineering competencies in the (then) IVC-SEP center, disciplines from five DTU departments were included, allowing us to unite expertise in areas such as thermodynamics, mathematical modelling, geology and geophysics. A consortium of companies from the energy and chemical sectors has supported the center over the years. Currently, 22 companies from four continents are members.

From day one, the philosophy of CERE has been to combine the primary disciplines – thermodynamics & transport, mathematics & mathematical modelling, geology & geophysics, recently also biotechnology – with other disciplines in order to solve broader problems in mainly petroleum, chemical, and biochemical engineering. While several important strategic areas have been identified (they are shown at CERE's website), we remain committed to allow faculty and researchers the academic freedom – and funding – to pursue new areas and directions. Another defining feature is combining experiments (at various scales), modeling-software, and dissemination. We always aim for development of generic models, concepts and measurements which can be of wide use and diverse applications. Also, the committed collaboration with our Industrial Consortium is a "must", and ideas from the Consortium continue to receive priority.

Obviously, we have seen a number of changes over our first 10 years. New faculty joined CERE, and new areas such as bioenergy and fundamental water studies have been integrated. We have also seen some faculty members apply their disciplines to a wider range of energy resources while some of the traditional fields have grown even stronger, e.g. carbon capture, utilization and storage (CCUS).

Some of these changes were based on strategic decisions, others were imposed by changing needs and interests of the faculty, society, and the industrial consortium. Fossil fuels continue to play a key role in CERE's activities. I expect this to continue. Even so, I also expect that the weight of bioenergy and CCUS in our portfolio will increase. Furthermore, fundamental studies in areas like electrolytes and water may also (as can be seen in this report) be developed further in the near future.

With the 10 years anniversary as a fitting occasion, this report offers a selection of topics from both the more traditional areas and from the new fields. From the oil & gas area, you may get updated on our continuing, strong collaboration with DHRTC (Danish Hydrocarbon Research and Technology Center). Also, several new developments within CCUS including the participation of CERE in 3D - a recently-funded large EU initiative.

Due to retire next year, Kaj Thomsen, expert in electrolyte thermodynamics, gives a special interview. The field of electrolytes will continue to be developed in CERE, as a major project funded by the European Research Council (ERC) was awarded to us in 2019. This five-year project is also presented.

Algorithms and computational aspects have always been strongholds in CERE, and will continue to be so as outlined in interviews with Associate Professors Wei Yan and Xiaodong Liang. Last but not least, recent findings in fundamental water studies are presented – another field of research which is expected to intensify in the coming years, as several new projects have been granted.

I hope you will enjoy the report. We will be looking forward to receiving any comments from you.
We also hope to see many of you during the forthcoming CERE Discussion Meeting 2020 (June 8-10), once again to be organized in partial synergy with the KT-Consortium Annual Meeting 2020 (June 9-11). Due to the COVID-19 situation, the CERE 2020 Discussion Meeting will be held on-line at a time and in a format which will be communicated soon to the member companies and other interested parties.

Professor Georgios Kontogeorgis,
Chairman of CERE
gk@kt.dtu.dk

Professor Georgios Kontogeorgis

INDUSTRY CONSORTIUM

A Summit of Industry-Academia Collaboration

Group picture from the joint day of CERE Discussion Meeting and KT Consortie Annual Meeting

The CERE Discussion Meeting is the annual event where members of the industry Consortium engage in discussions with the staff of the center. As usual, industry attendance was high - no less than 25 industry participants, representing corporations headquartered in 9 different countries. The three-day program included sessions on thermodynamics; CO_2 capture and electrolytes; petroleum applications; CO_2 storage and underground processes; The Synferon project (on fuel-from-biomass); and on joint projects with the Danish Hydrocarbon Research & Technology Center.
For the second consecutive year, the last day of the Discussion Meeting was co-organized with KT-Consortium, a cross-center activity at DTU Chemical Engineering. The KT Consortium is an industry-academia collaboration where members are provided networking opportunities and state-of-the-art methods and tools for chemical and biochemical engineering.

The CERE Discussion Meeting 2019 was held at Marienlyst Conference Center, Elsinore, June 11-13.









Facing the challenge of electrolytes

Freddy Garcia, Total

Mr. Freddy Garcia, Total: "We often tend to go around the problem when we see electrolytes formed (...). It would be better to have the tools for facing these problems head on."

Total, a long-standing CERE industry Consortium member, is one of the world's largest energy corporations. Its in-house Research & Development infrastructure spans the entire development process from laboratory testing to industrial scale production.

Mr. Freddy Garcia heads the Process Thermodynamics and Simulation group in Paris.

"This is my first CERE Discussion meeting. I am looking forward to the scientific presentations and to catch up on the latest developments within thermodynamic modelling. I am especially looking for areas where we and CERE have common interests."

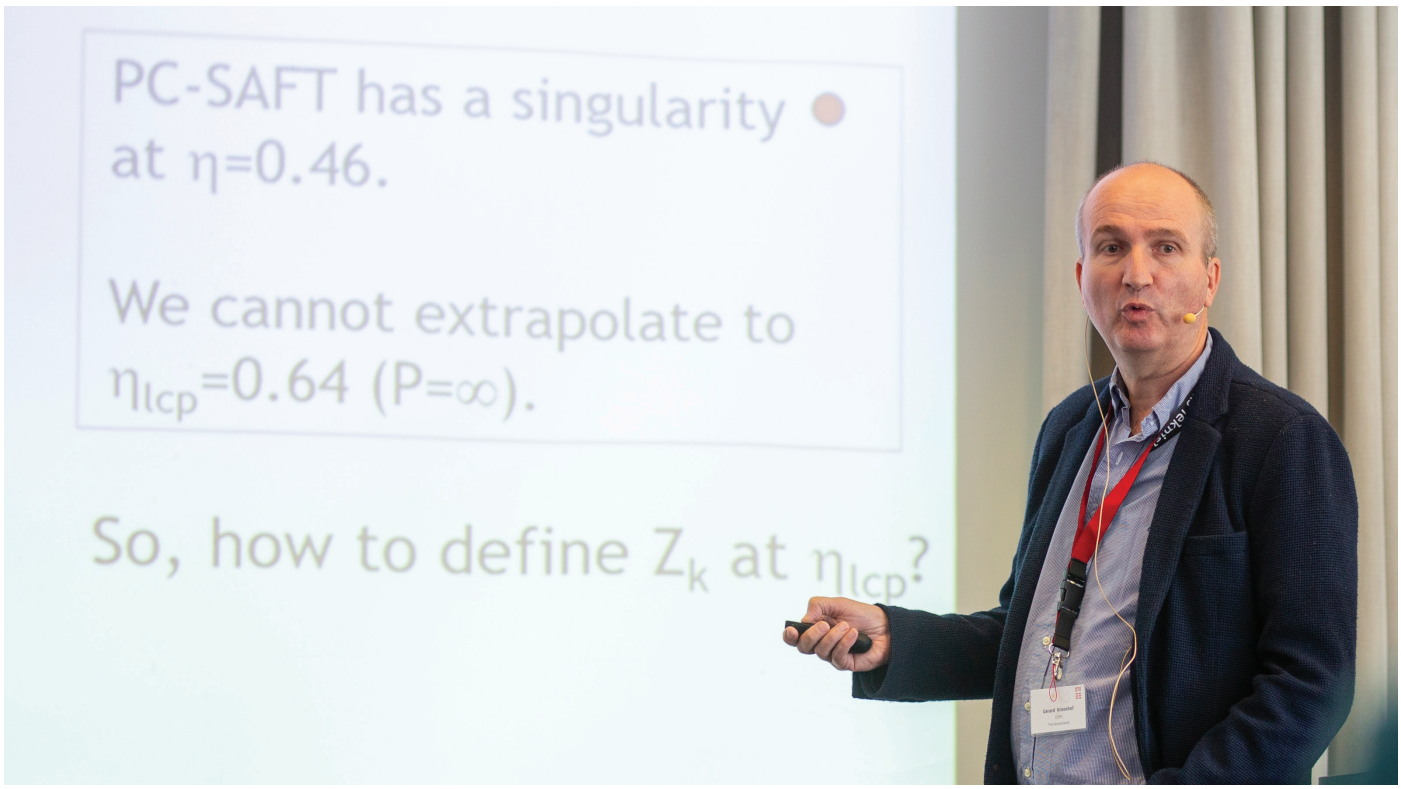
One such area might be electrolytes, Mr. Garcia elaborates:

"CERE is doing quite a lot of interesting work on electrolytes. We meet electrolytes in various contexts at our production facilities, but the current tools for modelling the behaviour of electrolytes can be limited for particular cases. Even though we often tend to go around the problem when we see electrolytes formed, sometimes this cannot be avoided. It would be better to have the tools for facing these problems head on."

Further, the academic content is not the only focus for the Total representative:

"The conference is a nice opportunity for meeting other industry representatives. It is always interesting to hear what other companies and the academia are doing. In general, I just try to keep an open mind when I come here."

Software supports sustainability of polymers



Gerard Krooshof, DSM

Dr. Gerard Krooshof, DSM: "Software from CERE helps us improving sustainability, e.g. through better modelling of polymer solubility."

Royal DSM has recently joined the CERE industry Consortium.

"We were attracted mainly by the high-quality software developed by CERE for various types of thermodynamic modelling, not least software based on PC-SAFT equations-of-state," says Dr. Gerard Krooshof, Senior Scientist in thermodynamics and colloid modelling at DSM.

Headquartered in The Netherlands, DSM is a global science-based company in nutrition, health and sustainable living. In respect to CERE, mainly the polymer activities are in play. DSM develops polymers for special applications e.g. in the automotive industry, electronics, paint and ink. Here, factors such as durability and stability are always important.

"Besides the ongoing developments for these various tasks, a growing trend is to also focus on the environmental properties. DSM is highly focused on sustainability. This adds an extra dimension to our research, and also leads to new requirements for software in modelling for instance of solubility of polymers," Dr. Krooshof explains.

After the company joined the CERE industry Consortium one year ago, software developed in CERE has been implemented.

"I have been pleased to see how the faculty at CERE has responded quickly to our queries," says Gerard Krooshof, while noting that he does not only attend the Discussion to discuss the current software applications:

"As in other parts of industry, we see a lot of focus on Big Data in biochemical and polymer engineering. In DSM, we are quite confident that this is more than just a hype. Also, we do have activities in quantum computation, DFT (Density Functional Theory, ed.) modelling and similar advanced simulation tools, and also try to bridge these emerging tools to existing chemical engineering tools. I was pleased to learn, that this is also being looked at in CERE."

"A bit on the same note, the new activities in CERE on the fundamental properties of water caught my attention. I must say, I am a bit sceptical when it comes to finding breakthrough applications of novel types of phase behaviour of water, but at the same time I am curious and look forward to following this. In any case, I find it encouraging that the group at DTU dares to engage in something which is a bit off the normal track."

A chance to discuss the fundamental issues

Even Solbraa, Equinor

Dr. Even Solbraa, Equinor: "I do not attend many conferences, but the CERE discussion meeting is a priority for me."

Equinor has been a CERE industry Consortium member for some 20 years. Most of the work has been under the umbrella of the CHIGP (Chemicals for Gas Processing) Joint Industry Project. Over the years, the Norwegian energy corporation has consistently sponsored Ph.D.'s in CERE. The most recent project was on subsea processing, which the company decided to pioneer six years ago.

"We see a large potential by doing the initial gas processing at the sea floor," explains Dr. Even Solbraa, Advisor in Oil and Gas Processing at Equinor. "The gas will always come up at high pressure. Traditionally, we have had to reduce the pressure significantly in order to process the gas at an offshore platform, and then later increase the pressure again to send the gas through the pipeline to an onshore facility. By processing the gas at the sea floor, we are able to maintain most of the original pressure. Thereby we save energy, and are able to produce the gas in a more sustainable manner."

For CERE, Even Solbraa has been the primary contact almost since the beginning of Equinor's membership. "My first Discussion meeting must have been in 2001 or 2002. I have always found these conferences well organized. I like the set-up with parallel sessions. This gives me the opportunity to choose, so I always hear presentations which interest me. I do not attend many conferences, but this one is a priority for me. I have always found the scientific content to be relevant for what we do in Equinor. Also, the attendance is a break for me from the day-to-day tasks. This is a chance to go deeper into the more fundamental issues."

Further, the Discussion meeting is a chance to scout new talent, Even Solbraa notes:

"Often, the next Ph.D. student is currently a Master student, and possibly present here. Actually, I also try to bring young people employed in Equinor here to introduce them to this community. I didn't manage that just this year, but hopefully that will be an exception."

BP (UK)
Calsep (DK)
Chevron (US)
DSM (NL)
Equinor (NO)
ExxonMobil (US)
Hess (DK)
IFP (FR)
KBC (UK)
Linde (DE)
MOL Group (HU)
National Oilwell Varco (US)
Neptune Energy (UK)
Nouryon (NL)
Petrobras (BR)
Schlumberger (US)
Shell (NL)
Sinopec (CN)
Total (FR)
Union Engineering (DK)
Welltec (DK)
Wintershall (DE)

The Consortium – our Strongest Asset

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

Furthermore, the center is supported by grants from several private companies. The strongest asset of CERE is the industrial Consortium.

Approximately 25 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.

CARBON CAPTURE

Next Level Carbon Capture

An ambitious European project is set to take carbon capture and storage (CCS) into industrial practice. CERE is a partner.

Eleven academic and industrial partners from six European countries are to develop and build a world-leading plant for capture of CO_2. When operational by 2021, the plant will be able to capture 0.5 metric tons of CO_2 per hour at the Arcelor-Mittal steel factory in Dunkirk, France. Of the total budget of no less than 19.3 million euro, the European Union's research and innovation program Horizon 2020 has supplied 14.8 million euro.

"This is the only project within carbon capture to receive support from the EU under that call, and obviously the competition for the grant was fierce. We are truly honoured to be a part of the winning consortium," says Associate Professor Philip L. Fosbøl. He and Associate Professor Nicolas von Solms are coordinating the participation of CERE in the project, which is called "DMX Demonstration in Dunkirk" (or "3D" for short).

Associate Professor, Philip I. Fosbøl

DMX is a carbon capture technology patented by IFP Energies Nouvelles, overall coordinator of the 3D project (and member of the CERE industry Consortium).

Contributing on compression and liquefaction

As DMX will be the capture method of choice, the CERE researchers will not be directly involved in developent of the actual capture of CO_2 but rather focus their attention at the subsequent steps.

"Obviously, carbon capture will only make sense if techniques to process the captured CO_2 further and store it underground are also in place. Our role in this project will be to contribute to solutions within compression and liquefaction of CO_2. These are the two first steps after the capture," Philip L. Fosbøl explains. "Also, we might contribute in the conditioning phase."

Conditioning basically means rinsing the produced CO_2 by removing various impurities such as H_2S, CO etc. Other partners will handle both the capture itself and the final stages involving transport and storage of the CO_2.
"We follow their activities closely and are already strongly engaged in coordination. This takes a lot of effort with that many partners, but will surely pay off. Even minor changes in the specifications of the captured CO_2 will have a severe impact during the later stages of processing. Only by being completely aligned will we be able to create a plant which is optimized in terms of energy use and thereby also cost-effective. This will be imperative for the dissemination of the technology to other parts of industry," Philip L. Fosbøl underlines.

Consistent CCS efforts in CERE

Dissemination of the developed solutions to industry is a high priority.

"As we are working directly with a number of industry partners, I am confident we will see a swift transferal of the results."

"According to the IPCC (...) we need to achieve negative emissions. Saying negative emissions is another way of saying Carbon Capture."
Philip L. Fosbøl, Associate Professor, CERE.

The CERE researchers will contribute with process simulations and optimization. Further, the results from CERE's participation will include a technical model describing the thermodynamics of the CO_2 compression and liquefaction processes. The model will be accessible in Aspen Plus to allow for easy implementation by industry and other stakeholders.

The fact that CERE is a partner in the top European CCS project, is more than a coincidence. While the political interest in CCS – and subsequently the interest from funding agencies – has fluctuated strongly, CERE has pursued carbon capture consistently. Especially has active participation in all major EU programs over the last two decades allowed CERE to maintain its level of research in the field.

"Our participation in these past CCS projects have opened doors and established many valuable contacts in

both academia and industry, and this has helped in positioning ourselves as an attractive partner," says Philip L. Fosbøl.

Danish commitment on climate

Looking a bit ahead, it seems likely that the CCS efforts at CERE can be extended further, since the Danish government is strongly committed to combating climate change.

"According to the IPCC, the world will need not only to get to zero carbon net emissions by 2050. If we are to preserve the present climate, we actually need to achieve negative emissions. Saying negative emissions is another way of saying CCS," notes Philip L. Fosbøl.

"Even with a full transition to renewable energy, we will still need to produce goods which are bound to emission of CO_2. We cannot just stop using steel, cement, medicine, paper and similar types of welfare goods which rely on processes which emit a noticeable amount of CO_2. Therefore, we will not be able to do without carbon capture. In other words, we should invest in CCS just like we invest in renewable energy technologies."

The 3D Project

3D project ("DMX Demonstration in Dunkirk") has a 19.3-million-euro budget over 4 years, including 14.8 million euro in European Union subsidies.

Coordinated by IFP Energies Nouvelles, the project involves 10 other partners from six European countries: Arcelor-Mittal, Axens, Total, ACP, Brevik Engineering, CERE, Cassco, RWTH, and Uetikon.

Associate Professor, Nicolas von Solms

Carbon Capture at CERE

For the CCS group at CERE, participation in the European 3D project ("DMX Demonstration in Dunkirk") is a flagship project. The group is currently in the process of hiring two researchers as a direct consequence of the 3D participation. "This will be a significant part of our efforts in the field over the coming 3 years," says Associate Professor Philip L. Fosbøl.

Still, the 3D participation is just a part of the activity on CCS at CERE. The group already has 5-6 researchers. Further, some 5-6 students are doing projects in carbon capture.

Notably, the group is active in several fundamental research projects. These include the use of ionic liquids (IL's) as solvents for carbon capture, and swapping CO_2 for methane in gas hydrates, respectively. Both of these projects are coordinated by Associate Professor Nicolas von Solms.

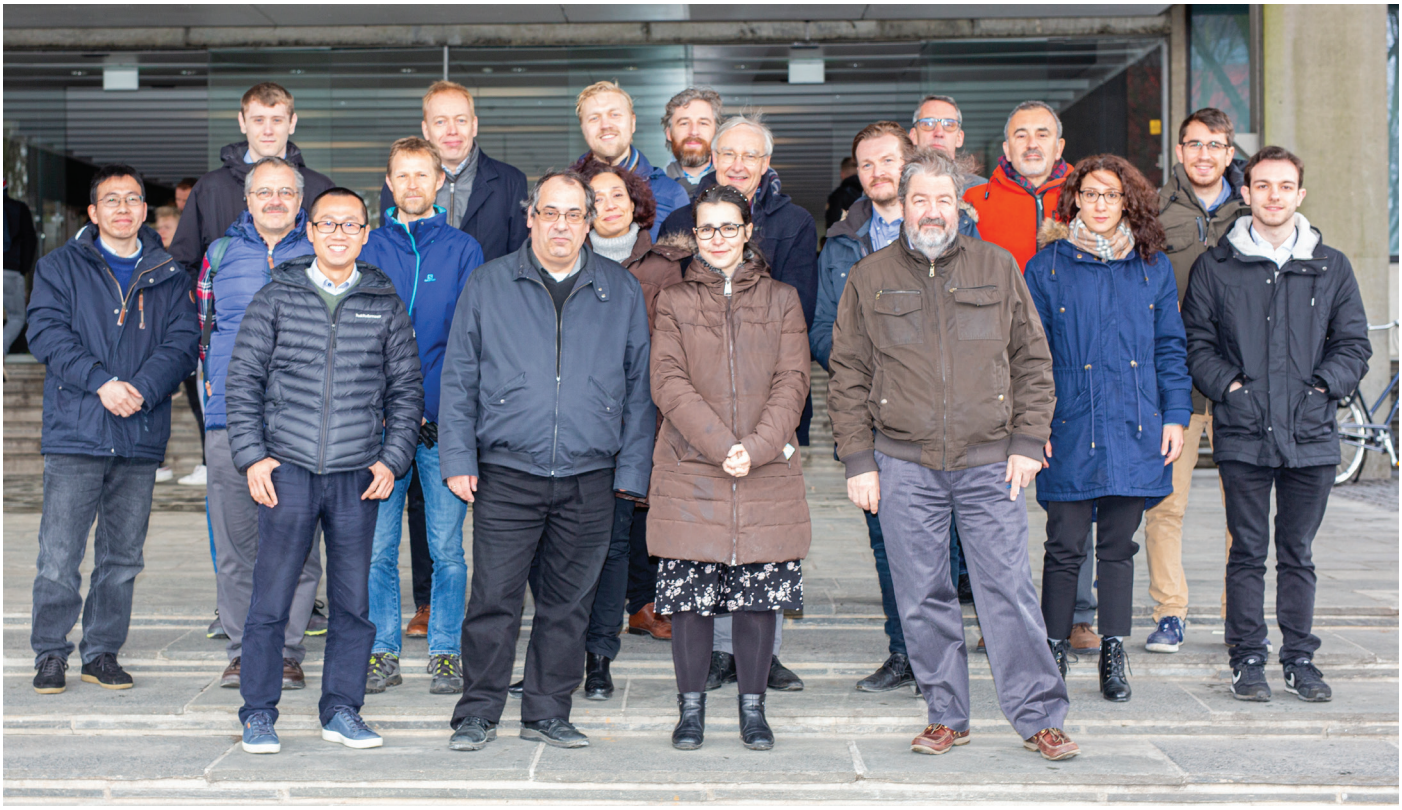
Further, carbon capture plays a role in three ongoing CERE projects with biogas as the common denominator. In the first project, MeGa-StorRE (Methane Gas Storage for Renewable Energy), methane is produced by removing CO_2 from the biogas.

In the second project, Bio Re-fuel, CO_2 is also removed from the biogas, but instead of methane, the end-product will be methanol. The third project, BioCO_2, focusses on utilizing the captured CO_2 as a valuable industrial feedstock.

All three projects are coordinated by Associate Professor Philip L. Fosbøl. The MeGa-StoRE and Bio Re-fuel projects were originally developed at DTU Mechanical Engineering, still a partner in both projects.

In 2019, support for several new projects was obtained; these include CO_2 sequestration, computational simulation of CO_2 storage, CO_2 capture by absorption, CO_2 capture, and carbon neutral energy by hydrate swapping.

Major Effort on Electrolytes



Funded by the European Research Council, an ambitious five-year CERE project is set to develop a new Paradigm in Electrolyte Thermodynamics.

Electrolytes are found in the vast majority of chemical engineering problems, yet their behaviour is relatively poorly understood. For instance, a survey by the European Federation of Chemical Engineers (EFCE) has pointed to electrolytes as lacking behind other areas of thermodynamic modelling.

A new project in CERE is aimed to change this
situation. The project "New Paradigm in Electrolyte Thermodynamics" is funded by the prestigious ERC
(European Research Council) Advanced Grant awarded to CERE Chairman Georgios Kontogeorgis.

"The overall target of the project is to obtain fundamental understanding of electrolyte thermodynamics and develop advanced engineering models, in form of electrolyte equations of state, for a broad range of electrolyte systems and applications. Indeed, whereas electrolytes are almost everywhere, major questions and exist. Some misunderstandings have remained for over 100 years, preventing real progress. It is the ambition of the ERC project to create a new paradigm, which will ultimately pave the way for the development of new engineering models for electrolyte solutions," Georgios Kontogeorgis states.
The ERC Advanced Grant is given to active researchers who "have a track-record of significant research achievements in the last 10 years" and who seek long-term funding to pursue a ground-breaking, high-risk project.

The 2.5 million EUR grant will allow for funding of about 10 PhD students and post-doctoral researchers over the coming five years.

Ready to look at controversial topics

Among the major topics will be the establishment of a database protocol and approaches for model development and validation, the comparison of the so-called primitive and non-primitive approaches in electrolyte thermodynamics, and the deeper understanding of the true validity and limitations of the Debye-Huckel theory and Born-type (solvation) effects. Further, the role of static permittivity effects especially for concentrated

"Whereas electrolytes are almost everywhere (...), some misunderstandings have remained for over 100 years, preventing real progress." - Georgios Kontogeorgis

electrolytes solutions and at high T/P conditions, the understanding of the balance of physical and electrostatic forces in electrolytic systems, and the combined use of extensive databases, advanced thermodynamic models and molecular simulation data will be investigated.

"We also expect to touch upon certain controversial topics such as the consideration of single ion activity coefficients and the role of the structure of water in electrolyte solutions. Despite the fundamental nature of the project, we will attempt to include industrial partners in the discussions and we believe that the results can be of interest to many member companies from both CERE Consortium and KT-Consortium," Georgios Kontogeorgis notes.

The project is in collaboration with University of Princeton (USA), NCSR "Demokritos" (Greece), and IFP Energies Nouvelles (France), member of the CERE industry Consortium. Moreover, CERE faculty members Xiaodong Liang, Nicolas von Solms and Hariklia Gavala are expected to participate in the project.

Models will be validated at their extremes

It is of particular importance to develop fundamental understanding that can lead to the development of generic models which can find applications in several of the areas where electrolytes are present including physical sciences e.g. chemistry, geology, material science, medicine, biochemistry and physiology as well as in many engineering fields especially chemical & biochemical, electrical and petroleum engineering.

"In this project, we attempt to go beyond the current state of the art and create a scientific foundation for studying and comparing diverse modern theories. We will validate the models at their extremes, i.e. conditions and situations never considered before in order to discover the frontiers of our understanding in electrolyte thermodynamics", Georgios Kontogeorgis explains, but is also quick to acknowledge the magnitude of this project:

"This is a risky, ambitious and crucial task, but a successful completion will have significant benefits in many industrial sectors as well as in environmental studies and biotechnology".

"This project has received funding from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme (grant agreement No 832460)".

Professor, Georgios Kontogeorgis

Affinity for Electrolytes

Widely recognized not least for his commitment to the Extended UNIQUAC model, Associate Professor Kaj Thomsen – to retire this summer – has every reason to be content with his contributions to the science of chemical engineering.

Kaj Thomsen would never introduce himself as "Mr. Electrolyte". When you are born and raised at a farm in Jutland, you just don't feel any need for using big words. So, we will take the fact that he only half-heartedly objects to the characterization as a kind of confirmation.

"Already as a kid, I took interest in the role played by salts in chemistry. I was inspired by seeing my father produce slaked lime. He prepared the mixture with great care, while warning me of the catastrophic consequences, should one err in the process," Kaj Thomsen recalls.

For centuries, slaked lime has been used for surface protection of buildings in rural areas in Denmark. It is a cheap and decorative method, but if you get the amounts and timing wrong, the mixture can actually explode. This is an example of how the presence of electrolytes – dissolved salts – can change the behaviour of solutions.

Energy resources engineering and numerous other chemical engineering applications involve electrolytes. Just to take one example, electrolytes are found in both formation and production water during oil and gas production. This often causes scaling in pipes when the solution is subjected to changes in temperature and pressure.

"Already as a kid, I took interest in the role played by salts in chemistry. I was inspired by seeing my father produce slaked lime."
Kaj Thomsen, Associate Professor, CERE.

A new method for parameter determination

As scaling potentially can plug pipes and other equipment and thereby induce vast economic losses, the energy resources industry takes great interest in modelling the behaviour of electrolytes. Kaj Thomsen joined the field in 1993, writing his master thesis and PhD thesis on the subject. As a candidate in chemical engineering, he was able to continue on this line at DTU in the group which is now a part of CERE.

"The first models had already been developed before I joined, in the 1980'ies, and taken into use in industry. However, the models were rather limited concerning the size of electrolyte systems which could be managed. This was a problem, as the real-life systems often are quite complex with many different ions present at the same time. My main contribution was to introduce a new method for determining parameters in this model. The limitation was removed so that more ions could be added to the systems," Kaj Thomsen explains.

Electrolyte solutions behave very differently from non-electrolyte mixtures. The presence of salts decreases water activity, which in turn will lower the freezing point and raise

the boiling point. Further, electrolytes will dissociate into cations and anions within the solution. These charged species will engage in electrostatic interactions on a far greater range than the common interactions between molecules. The interactions cannot be modelled with conventional models used for fluids.

Activity coefficient models stand strong

Currently, two approaches to modelling of electrolyte solutions exist. A relatively new approach is to develop electrolyte equations of state (EoS), typically by building on an already existing EoS able to account for the short-range interactions. CERE is highly active in this respect, and Kaj Thomsen contributes to several projects. Still, his main interest over the years has been the other approach, which is known as activity coefficient models.

"Some have claimed activity coefficient models to be outdated, but in my view, they are still standing strong. The EoS based models are certainly interesting, but because they use the ideal gas state as reference – a state far from electrolyte solutions – a lot of extrapolations are needed. Therefore, activity coefficient models are the standard method and will probably remain the standard for some time," says Kaj Thomsen, pointing to some of the current practical applications:

"Take fields such a carbon capture or optimization of lithium production. I don't think anybody would suggest using EoS based modelling at this stage."

Elegant solution to a tricky problem

While Kaj Thomsen has contributed to several activity coefficient models, his name is mainly tied to the Extended UNIQUAC. In this model, salt solubility data are part of the parameter regression.

Originally, the implementation of Extended UNIQUAC was halted because the model had difficulties in managing systems with mixed solvents. In other words, if both water and another solvent was found in a given mixture – as is often the case in chemical engineering – the model had shortcomings. Some would tackle this problem by introducing an extra model, but in 2000 Kaj Thomsen suggested how the problem could elegantly be overcome within the model. In the following years he and co-workers in CERE managed to prove the soundness of his idea, resulting in convincing publications in 2004-2005.

Today, Extended UNIQUAC is considered a reliable model for electrolyte systems for temperatures up to 383 K, covering a wide range of practical applications, and it has been implemented in a number of commercially available simulators.

Modelling of electrolytes is still underdeveloped

Besides Extended UNIQUAC, widely used activity coefficient models are the e-NRTL, Pitzer, and MSE (Mixed Solvent Elecrolyte). Further, a number of EoS based models have emerged. Some ten years ago, CERE researchers in collaboration with industry partners compared a range of models. This exercise did not produce a clear winner, Kaj Thomsen explains:

"We saw different models being better under different conditions. In other words, you cannot just take a model from the shelf. You need firstly to produce a fair amount of data. Then, we will be able to determine which model will be the best for your problem."

In 2010, a survey by the European Federation of Chemical Engineers (EFCE) pointed to electrolytes as lacking behind other areas of thermodynamic modelling. The survey was based on answers from engineers in chemical, pharmaceutical and petroleum industry to a questionnaire. "Despite the progress made, I think it is still fair to say that modelling of electrolyte systems is underdeveloped," Kaj Thomsen admits.

"Fortunately, CERE will have an opportunity to do even more in the field, thanks to the European Research Council Advanced Grant 2018 awarded to Professor Georgios Kontogeorgis for his project on "New Paradigm in Electrolyte Thermodynamics"."

Visiting Professor in Xining, China

Although Kaj Thomsen officially retires by June 2020, he will not leave chemical engineering. Until the end of August 2023, he continues as Visiting Professor at the Quinghai Institute of Salt Lakes, Chinese Academy of Science (QISLCAS). This includes teaching electrolyte solution thermodynamics at QISLCAS in Xining, China.

Further he may have a role to play at CERE as emeritus.

"We haven't really talked about this yet. But actually, I do have some ideas."
In any case, the enthusiasm of Kaj Thomsen when it comes to electrolytes has not been dampened over the years, on the contrary:

"The more I have studied electrolytes, the more have I found them to be interesting. Electrolytes are present in nearly all chemical engineering fields – and even in biology. Just think about it: each and every biochemical reaction taking place in our bodies actually involves electrolytes!"

OIL AND GAS APPLICATIONS

Towards Cleaner Offshore Oil Production

Postdoc Tian Wang

In collaboration with DHRTC, new efforts in CERE will address innovative methods for optimizing the cleaning of water produced during oil and gas exploration.

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.

"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 rinsed as it contains various impurities such as oil drops, solid particles, corrosion inhibitors and other chemicals," explains Associate Professor Alexander Shapiro, carrying out the petroleum related research and heading petroleum education activities in DTU.

The water already undergoes cleaning, but the upcoming projects are intended to take things to a new level. "As academic researchers we are keen to develop entirely new concepts in collaboration with the colleagues from DHRTC, and our ambition is to remove well above 99 per cent of the impurities," says Alexander Shapiro.

Greener profile in DHRTC projects

Six years ago, the Danish Hydrocarbon Research and Technology Centre (DHRTC) was born, initiated by a donation from Maersk Oil (later acquired by Total). Since, many petroleum activities in CERE have run in collaboration with and support from DHRTC.

"We have a natural division of work, as DHRTC is directly focused on development of petroleum production in the Danish part of the North Sea, while we in CERE do not have the same limitation but obviously have overlapping interests," says Alexander Shapiro.

Currently, three PhD and one Postdoc projects at CERE are funded by DHRTC, which was founded in 2014 with a ten-year horizon.

"The collaboration has been extensive all along, and still is. If I should point to one significant change, here as DHRTC has passed its halfway-mark, it would be the greener profile. From the outset, DHRTC was very much focused on maximizing production from the Danish fields – in particular, on enhanced oil recovery (EOR). This is still a strong focus, but the desire to develop more environmentally benign techniques and practices has become much higher on the agenda during the last few years," Alexander Shapiro notes.

Producing oil and rinsing water

Extracting oil and gas from the underground and cleaning the water may sound like two completely different topics, but that is not at all true: "Through our involvement in EOR projects over the recent years, we in CERE have acquired a deeper understanding of mechanisms involved in transport of oil and brine in porous media and similar processes, which all are relevant to filtering techniques for offshore water cleaning. Chemistry of oil, saline water and additives has also been studied. From an academic viewpoint, EOR and cleaning of the produced water are very similar. We are therefore entering the field with confidence, and are involved in

defining several interesting projects together with DHRTC."

The relevant insight has to a large degree been obtained in the projects related to so-called "smart water-flooding", involving a range of CERE faculty members from different DTU departments, and industry partners. This strategy in oil production involves injection of water with a modified salinity. The purpose is to extract additional oil from a reservoir. Several possible physical and chemical mechanisms that might be responsible for success of smart water injection have been investigated in these projects.

"From an academic viewpoint, Enhanced Oil Recovery and cleaning of the produced water are very similar."
Alexander Shapiro, Associate Professor, CERE.

Practical experiments are required

Especially an ongoing project conducted by Postdoctoral researcher Tian Wang, CERE, is relevant to both EOR and water rinsing applications. Tian Wang and co-workers investigate how brines with different salinities can mobilize oil drops in a porous rock. The project involves extensive microfluidics experiments: study of oil droplets in thin capillaries, how these droplets move and interact with each other.

"This is an area where practical experiments are very valuable. An oil drop will either pass narrow pores and constrictions and, eventually, get recovered, or it will not. In either case you obtain very direct information in experiments with a single thin capillary with a constriction. If we could recover just one drop more from each cubic centimetre of reservoir, this could give a large increase of the oil recovery," says Alexander Shapiro, supervising the Postdoc project jointly with Advisor Simon I. Andersen, DHRTC. Simon Andersen is also leading the produced water cleaning program at the DHRTC, in the framework of which the microfluidics experiment will hopefully continue.

Further, interaction of oil droplets with saline brine and chemicals does involve a lot of applied thermodynamics which is a longstanding core area for CERE. Here, a range of CERE researchers possess an expertise, not least Associate Professors Kaj Thomsen and Xiaodong Liang.
"Their work has inspired ideas for filtering techniques which will be investigated in the upcoming projects, possibly leading to new inventions," says Alexander Shapiro.
Last but not least, CERE has conducted research on use of bacteria in EOR. It was attempted to apply the same types of bacteria to cleaning of the oil spills. Then the bacteria may be filtered out, similarly to the previously studied microbial enhanced oil recovery. A collaboration between DHRTC, CERE, and DTU Environment is envisaged.

A focus on deep reservoirs

On the more traditional side of the collaboration with DHRTC, several joint EOR projects are ongoing at CERE.

The largest project focusses at the Lower Cretaceous layers in the Danish part of the North Sea. While exploration to date has been concentrated on the younger Upper Cretaceous layers, also the Lower Cretaceous layers contain substantial oil and gas reserves. Several ongoing projects in CERE, all undertaken in collaboration with and sponsored by DHRTC, focus on these deep and complex reservoirs.

As the Lower Cretaceous geology is dominated by low-permeable chalk, it has been proposed to produce the reservoirs by gas injection. This is the subject of a project by Postdoc Duncan Paterson with Professor Erling H. Stenby and Associate Professor Wei Yan as supervisors. Injected gas can achieve different extents of miscibility with reservoir oil and reduce the residual oil saturation. If complete miscibility could be obtained, the injected gas would recover 100 % of the oil.

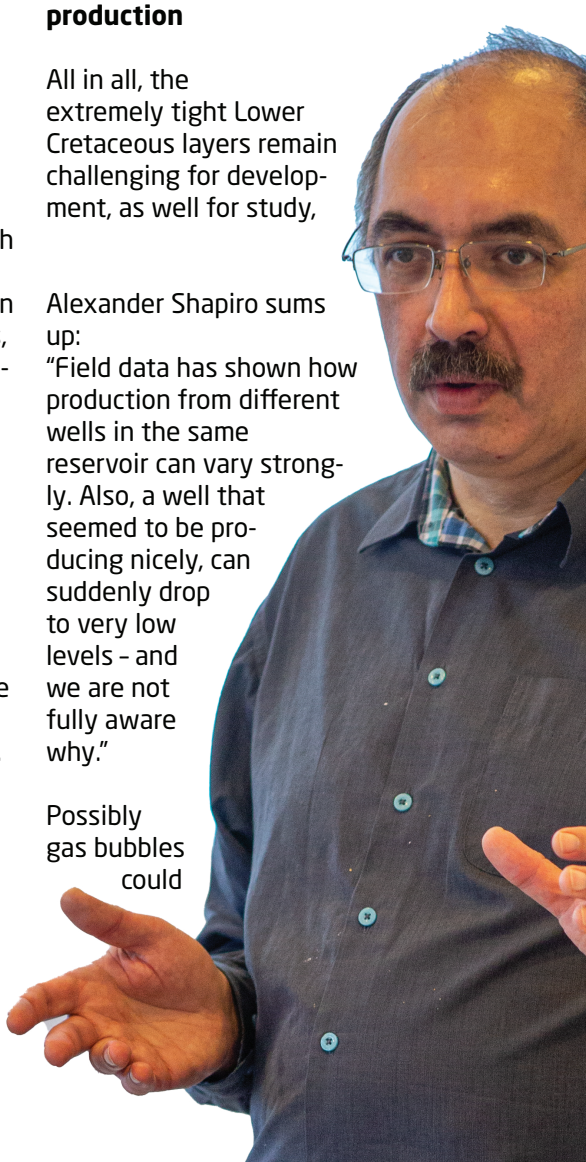
Another key topic is the influence of porous media on phase behaviour. Field observations suggest that the saturation pressure in tight formations may change dramatically. Therefore, it is expected that the extremely low permeable Lower Cretaceous rock may influence the phase behaviour of the reservoir fluid, and this is the subject of the project by Postdoc Diego Sandoval with Associate Professor Wei Yan and Professor Erling H. Stenby as supervisors. The project builds on experience from a recent shale project with ConocoPhillips.

Innovation is key to further Danish production

All in all, the extremely tight Lower Cretaceous layers remain challenging for development, as well for study,

Alexander Shapiro sums up:
"Field data has shown how production from different wells in the same reservoir can vary strongly. Also, a well that seemed to be producing nicely, can suddenly drop to very low levels – and we are not fully aware why."

Possibly gas bubbles could



be created in the oil as the reservoir pressure drops with oil production. These bubbles may work as "props", plugging the pores and hindering the production. A project in CERE carried by PhD Student Wael Al Masri and supervised by Alexander Shapiro will investigate this hypothesis.

Of the Lower Cretaceous fields in the Danish part of the North Sea, the Valdemar Field is believed to contain the largest amounts of oil and gas. However, it remains clear, that only small fraction of oil may be recovered from Lower Cretaceous fields without extensive scientific and technological progress.

"This can be said for all the fields in the Danish part of the North Sea," Alexander Shapiro notes, summing up: "The only way Denmark will be able to produce more oil is through innovation. We know this is difficult to carry out at a time with low oil prices. Should, however, the scene change, we will surely be ready to contribute on the academic side."

Putting the Squeeze on Super-tight Chalk

Leonardo Meireles

A rock-mechanical mechanism previously unknown in chalk has been developed through CERE-DHRTC collaboration. The discovery raises hope for better oil recovery in chalk reservoirs and better oil content evaluation of Super-tight Chalk.

Much like squeezing a toothpaste container, oil sitting in a chalk reservoir can be forced to leave its shelter with the correct composition of the brine used for water flooding. This is the possible implication of a previously unknown rock-mechanical mechanism developed by CERE researchers in collaboration with Danish Hydrocarbon Research and Technology Centre (DHRTC).

The mechanism has been interpreted in a PhD study by Leonardo Meireles, CERE, now Postdoc at DTU Civil Engineering.

"Our studies show how the interplay between charged inner surfaces of chalk contributes to the mechanical elasticity of the rock. This is well-known in clays but has only recently been shown in chalks. The discovery implies, that it will be possible to soften the pores of the chalk by applying brine with the right composition. As the chalk softens, it will contract and we can get the desired "toothpaste container" effect," explains Professor Ida L. Fabricius, heading the group.

Things are not all that simple though, as a too strong contraction of the chalk will have adverse consequences – the structure can collapse to an extent where production becomes impossible. So, further studies and a generally cautious approach is recommended. But still, the discovery can be good news for future exploitation of certain reservoirs, which are known to contain large hydrocarbon reserves while currently being uneconomical to produce.

An unexpected finding

The results by Leonardo Meireles and Ida Fabricius originate from a collaboration with Senior Scientist Michael Welch at DHRTC on advanced water flooding of Upper Cretaceous chalk. Possible applications of the new rock-mechanical knowledge will be investigated with an eye to enhanced oil recovery (EOR) in the Dan field. The Dan field was the first Danish field to be produced, and has also been the largest field by a great margin when it comes to the total amount of produced oil over the years. Still, the return on investment for the operators has been relatively small, because the chalk in the Dan field is very tight, making production more costly and difficult.

"As so often happens in research, the most interesting findings come from ideas you didn't think of in advance."
Ida L. Fabricius, Professor, CERE.

Lower Cretaceous chalk layers in the Danish part of the North Sea contain substantial oil and gas reserves, but also a varying content of clay, which lowers oil flow, so these reservoirs have till date been underdeveloped. Thus, DHRTC decided a few years ago to fund a series of projects on the Lower Cretaceous formations. A number of these projects are conducted in collaboration with CERE.

"While the new rock-mechanical mechanism has been developed as a part of our collaboration with DHRTC on the Upper Cretaceous formations, the presence of charged particles can have significant effect on our evaluation of Lower Cretaceous chalks in an unexpected way, because traditionally only clay has been seen as charged.

This was not a part of our original thinking. As so often happens in research, the most interesting findings come from ideas you didn't think of in advance, but develop somewhere along the way," Ida Fabricius notes, continuing:

"It may sound boring to some, but I actually believe we can attribute this and other findings to having a systematic approach. To paraphrase, we will not dive straight into the sea but map the coastline first. While this approach is quite laborious, it very often does pay off in the end."

Inspired by tiny crystals

The Lower Cretaceous layers are older than the Upper Cretaceous layers, and characterized by even tighter chalk – so truly super-tight chalk. Also, this chalk has tinier crystals than seen in the Upper Cretaceous formations.

"It is quite possible that we noticed the charged particle mechanism because of the very tiny crystals in the Lower Cretaceous core samples, but that the same effect is also present in other fields in the Danish part of the North Sea," says Ida Fabricius.

The new geological knowledge may also come to use in fields outside oil and gas applications, Ida Fabricius ends:

"The core interest in our group is the fundamental mechanisms involved in chalks and similar types of rock.

Obviously, oil and gas applications are the focus of our collaboration with DHRTC, but we are always happy to see applications in other fields - an example could be in geo-technical applications – just as discoveries in other fields have often helped in hydrocarbon applications."

Ida Lykke Fabricius

"I could, rhetorically, ask whether you would rather have a fast answer or a correct answer?"
Xiaodong Liang, Associate Professor, CERE.

Algorithms for Flash and Beyond

While decades of ground-breaking development of algorithms for flash calculations continues at CERE, new areas such as Density Functional Theory are on the rise.

Founded at DTU by Michael Michelsen, and spearheaded by him over several decades, CERE has algorithms for flash calculations as a long-standing top priority. Mathematical tools able to predict the phase distribution of a mixture with known composition under different temperature and pressure scenarios have always been highly useful to both the petroleum industry and in several other chemical engineering applications. Today, the area is led by Associate Professor Wei Yan.

Duncan Paterson (today with Linde) worked on flash computation and equation of state (EoS) modelling for compositional thermal simulation of flow in porous media under Wei Yan's supervision. Apart from research on thermodynamic modelling and composition simulation, he has made several important contributions to flash calculation algorithms for multiple phases and for various specifications. He has received the Springer Thesis Award for this PhD research. A major contribution by Duncan Paterson is the formulation of a RAND-based flash framework. The framework radically changes performance of flash calculation and is particularly suitable to multiple phases. Besides, the framework allows calculation of reaction equilibrium together with phase equilibrium. Duncan Paterson successfully applied the framework to multiphase flash with various flash specifications, and implemented it in a commercial simulator.

Associate Professor Xiaodong Liang

"The methodology is demonstrated to be robust for a number of mixtures," notes Wei Yan, continuing: "The conventional isothermal flash framework is cumbersome when dealing with more than two phases. A new framework developed by Duncan Paterson addresses this issue. It provides a more robust and structured solution to multi- phase flash, and further- more the possibility of si- multaneous calculation of reaction equilibrium."

Extension to reactions

In a PhD project by Christos Tsanas (today with IFP Energies Nouvelles), a new methodology capable of calculating phase equilibria for complex challenges in both chemical industry and energy engineering applications has been developed. The proposed solution is a hybrid of two different non-stoichiometric approaches. In the first of the two methods, the Lagrange multipliers method, successive substitution is employed to solve a modified set of equations originating from the Lagrangian conditions at the minimum. In the second method, the modified RAND method, one of the Lagrangian conditions is linearized around the current estimate of mole numbers. Composition derivatives of fugacity or activity coefficients are utilized to achieve quadratic convergence.

"The combined method developed by Christos Tsanas proved applicable all the way from simple one-reaction ideal systems to highly non-ideal electrolyte mixtures with speciation reactions and solids. Both algorithms were able to converge to the equilibrium solutions. Considering CPU time and a reasonable number of iterations, the method is demonstrated to be efficient and robust," Wei Yan comments.

"Christos' work will benefit many modelling and simulation tasks involving reactions, including our ongoing research on geological CO_2 storage involving geochemical reactions."

The speed versus accuracy trade-off

Besides development of entirely new methodology, a strong focus in the group is to improve the efficiency of

Christos Tsanas

algorithms in order to limit the necessary resources for computing while also allowing for faster results. Especially for the more advanced thermodynamic models such as CPA (Cubic Plus Association) and PC-SAFT it is a reoccurring complaint from industry, that flash calculations are too slow.

Duncan Paterson showed that volume-based thermodynamics can improve the speed for CPA and PC-SAFT in compositional simulation to a few times slower than cubic models.

"I am aware that some industry colleagues will argue this is still too slow, and therefore CPA and PC-SAFT will not be applied. I could then, rhetorically, ask whether you would rather have a fast answer or a correct answer? Especially when we are talking about complex mixtures, asphaltenes and other tricky problems we know that the cubic equations of state do have their limitations," Associate Professor Xiaodong Liang from the group comments.

Density Functional Theory

Before joining DTU in 2011, Xiaodong Liang had worked in development of thermodynamic models and algorithms for a commercial process simulator for more than 4 years. At CERE, he did his PhD study on modelling of various chemical engineering problems, involving both PC-SAFT and PT flash calculations. He also began assisting the PhD summer course – highly praised by industry consortium members – on advanced thermodynamic modelling and PT flash calculations.
"I would like to add that Michael Michelsen is still highly active. We have regular communications and develop fresh ideas together," notes Xiaodong Liang.

One such idea was explored 2016-2017 in a project on Density Gradient Theory (DGT), a special version of Density Functional Theory (DFT).

"Starting from a short note by Michael Michelsen, we had a very productive collaboration on developing algorithms and approximation methods based on DGT. One significant aspect was that we proposed to solve a second-order boundary value problem by a minimization method using the collocation method developed by Michael and co-authors in the 1960'ies and 1970'ies."

"The methodology is demonstrated to be robust for a number of mixtures," Associate Professor, Wei Yan, CERE

Another journey about to begin

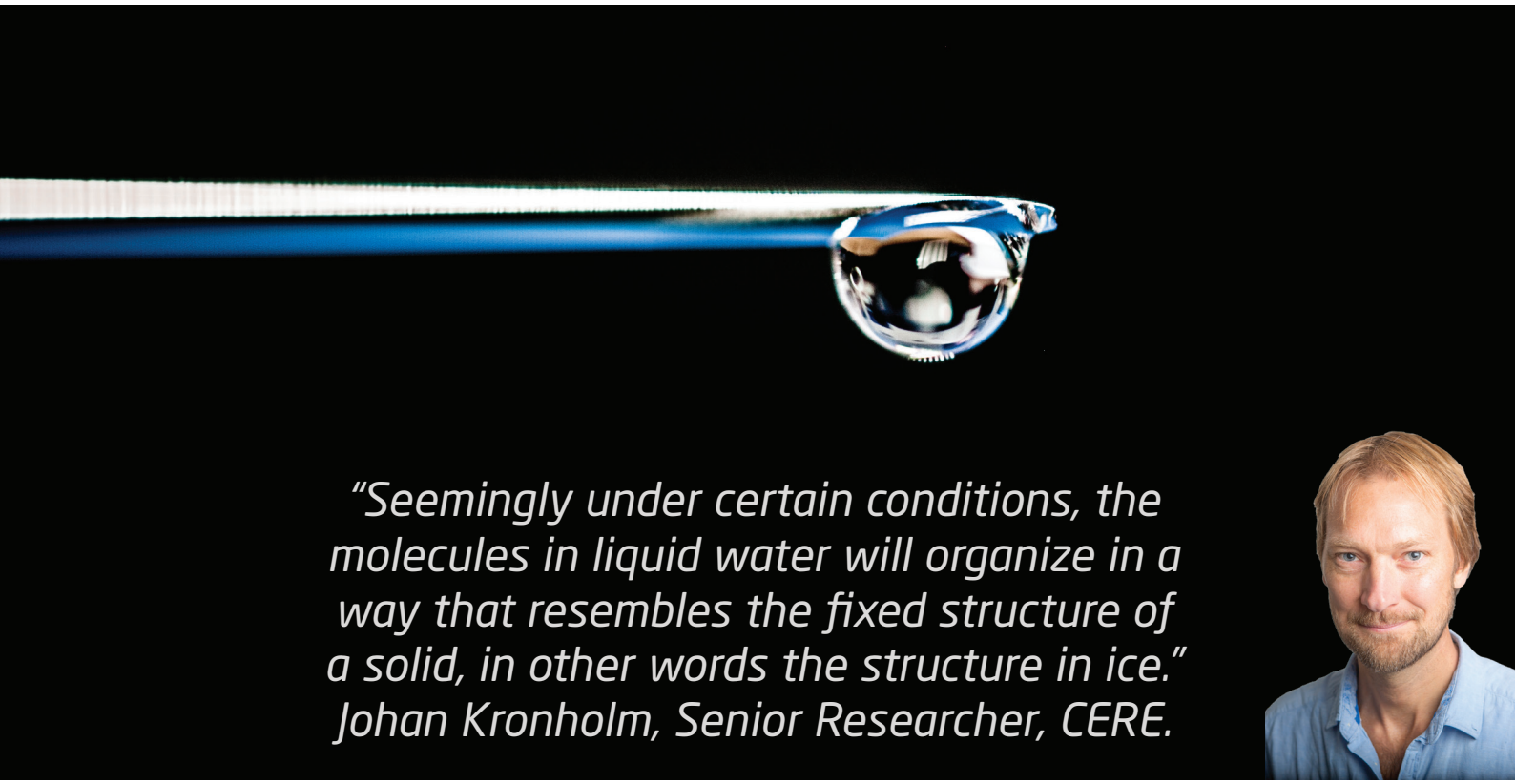
Remarkably, the group managed to reduce calculation time from 20 minutes down to just 0.01 seconds.

"In other words, we reduced calculation time by a factor of around 10,000. I do consider this one of our most significant achievements in recent years," says Xiaodong Liang.

However, the project also revealed that DGT is not appropriate in all situations, and with support from DTU Chemical Engineering, a new PhD project on a more general Density Functional Theory (DFT) framework has recently been initiated. While results from this project and other efforts on DFT will have to wait for future annual reports from CERE, Xiaodong Liang can safely conclude Michael Michelsen's legacy to continue:

"Significant progress has been made on developing DFT from scratch. It is always exciting to receive emails and notes from Michael, usually with brilliant ideas on how to solve new or existing problems. For instance, Michael recently sent us a note on critical point of associating fluids with the CPA equation of state – another exciting journey is about to begin!"

Associate Professor Wei Yan



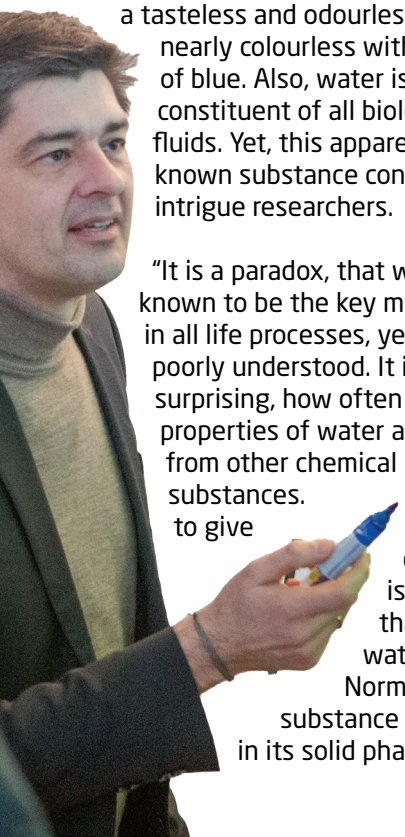
"Seemingly under certain conditions, the molecules in liquid water will organize in a way that resembles the fixed structure of a solid, in other words the structure in ice."
Johan Kronholm, Senior Researcher, CERE.

Johan Kronholm

The Intriguing Water Molecule

All biological processes, and practically all industrial processes, involve water. Yet, this seemingly simple molecule continues to surprise.

Water, H_2O, is a polar inorganic compound that is at room temperature a tasteless and odourless liquid, nearly colourless with a hint of blue. Also, water is the main constituent of all biological fluids. Yet, this apparently well-known substance continues to intrigue researchers.



"It is a paradox, that water is known to be the key molecule in all life processes, yet remains poorly understood. It is surprising, how often the properties of water are different from other chemical substances. Why, just to give an example, is ice lighter than liquid water? Normally, a substance is heavier in its solid phase than as a liquid," says Senior Researcher Nikolaj Sorgenfrei Blom, based at DTU Chemical Engineering and heading fundamental research on water in CERE.

The efforts were initiated in 2015, when Nikolaj Sorgenfrei Blom and Senior Researcher Michael Bache – at that time with DTU Nanotech - saw common interests.

"Nikolaj worked in biological research, while I was studying microfluidics. Since, I have come to realize that what I was really studying at that time was actually not so much nanotechnology, but rather the fundamental behaviour of water molecules," says Michael Bache.

"Water is by far the most commonly used solvent in chemistry and chemical engineering. This fact alone would justify our interest, but actually the possible applications of new fundamental findings from water research span across numerous sectors."

The Italian connection

The common interest was fuelled further, as Professor Livio Giuliani obtained an Otto Mønsted grant for a stay as visiting professor at DTU. He is a pioneer in the field of bio-resonance and quantum biology. In 2014, Professor Giuliani and co-workers had showed an effect of exposure to low-frequency magnetic fields on certain pathogens that are known to cause critical conditions in cystic fibrosis (CF) patients. The study, published in Future Microbiology, attributed the effect to subtle changes in the pathogens' water molecules – hindering the ability of the pathogens to form biofilms.

Inspired by this and other international studies, Nikolaj Sorgenfrei Blom designed a water research project with possible health care applications. By 2017, the project obtained funding from the VILLUM foundation. Also, a regional EU grant for investigating water-modifying devices was obtained, and the group was established at DTU Chemical Engineering as a part of CERE.

"Many departments at DTU are active in water research, but it was natural to establish the group as a part of CERE, since Professor Georgios Kontogeorgis, Chairman of CERE, has a longstanding interest in modelling of water for chemical engineering purposes," notes Nikolaj Sorgenfrei Blom.

Water as a liquid crystal

One year later, in 2018, the VILLUM foundation granted support for a related project, which allowed the addition of Senior Researcher Johan Kronholm to the group.

The bold ambition in the project of Johan Kronholm is to contribute to a better understanding of the fundamental nature of water. For instance, a hypothesis featuring a fourth phase for water – in between solid and liquid – has caught momentum in the international scientific literature.

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

A fourth phase of water could be regarded as a gel or as a liquid crystal.

"It is quite possible that application of electromagnetic fields with certain frequencies may shift the balance between this type of structured water, and the normal, less structured water. It would obviously be highly desirable to know the mechanism. Firstly, because this would be highly helpful for further development and optimization of existing water technology equipment, and secondly, because this understanding could open doors to many other applications," according to Johan Kronholm.

Customers are happy, scientists frustrated

Several nations struggle with water scarcity, and many – if not all – with severe threats to the quality of water from various types of pollution. While this is obviously a challenge, it also represents billion-dollar business opportunities. Not least is Danish industry well positioned through long traditions for water and environment technology.

"The growth potential in water technology can hardly be overestimated. For Denmark, the prospects could be similar to or even greater than those of wind turbines," notes Nikolaj Sorgenfrei Blom.

"So large is the potential, that anyone with innovate ideas really should feel encouraged to pursue them," says Michael Bache, half-smilingly adding: "Even ideas that some would call wacky could actually be worth considering."

The members of the group at CERE acknowledge this to be a sensitive subject. Usually, we would expect science to first propose a mechanism, and then industry to develop the appropriate equipment. But this is not always the route in water technology.

"We see several start-up companies manufacture equipment for which they cannot explain the mechanism properly. As long as the equipment works – for instance by removing carbonate scaling, preventing biofilm formation or solving other major water related problems – the customers will of course be happy. But scientists will be upset!" says Nikolaj Sorgenfrei Blom.

Ending the deadlock

Rather than being upset, the water group at CERE seeks to embrace such new types of equipment and pursue satisfactory explanations to their effect.

"Just like the rest of us, the companies would like to be able to understand the function of their "miraculous" products. Both as selling points, and as a means to optimize products," notes Michael Bache.

The search for mechanisms behind various types of water modification by magnetic fields, ultrasound, electromagnetic waves and other methods involves extensive experiments.

In this way, the group hopes to end the deadlock between on the one side conventional scientists, and on the other side proponents of the existence of unfounded "mystic" effects, Nikolaj Sorgenfrei Blom concludes:

"By no means are we suggesting the existence of black magic, but we want to keep an open mind. We acknowledge that we are not yet at the point of understanding all aspects and properties of water. Improving this understanding could lead to new and better ways of water treatment and transformation of water-based processes. In other words, largely any industrial or natural process could potentially be optimized."

Water research continues

Two projects funded by the VILLUM Foundation have taken water research at CERE to new heights. While one of these projects ran out by 2019, and the second will finish in 2020, activities will continue in various other projects. For instance, the Maritime Fund and ship owners Molslinjen have jointly provided funding and support for a project on limiting NOx emissions from ferries through electromagnetic treatment of fuel. Senior Researcher Michael Bache, CERE, is involved in the project which is conducted in collaboration with DTU Aqua.

Postdoc Humbul Sulemann

Girls in Science Day

40 high school girls visited CERE on 2 October, as part of the DTU event "Girls' Day in Science". In the workshop format and with "Science behind climate change" as a common denominator, CERE researchers would guide their guests through the latest developments in carbon capture and storage (CCS), energy storage, gas hydrates, and water science.

Associate Professor Philip Fosbøl introduced the overall topic of the day, challenging the girls in a quiz on CO_2 emission facts. He went on to explain to the engaged audience how science can contribute to fighting climate change.

Next on the agenda was a tour of the CERE labs, including a range of presentations from researchers. Senior Researcher Nikolaj Blom, Postdocs Humbul Suleman and Susana Almeida, PhD students Yingjun Cai, Meng Shi and Lucas Corrêa, and Research Assistant Athanasios Varsos presented their work on water science, lithium batteries, gas hydrates, and CO_2 capture.

The day was hosted by Researcher Teresa Regueira and Research Assistant Randi Neerup. The two organizers were assisted by Postdocs Tian Wang and Zahra Nickmand and by PhD student Hadise Baghooee.-

The photograph shows Nicolas von Solms amidst the separation technologies group of the University of Stellenbosch.

Invited Seminars in South Africa

Associate Professor Nicolas von Solms, CERE, was invited to give research seminars at two universities in South Africa.

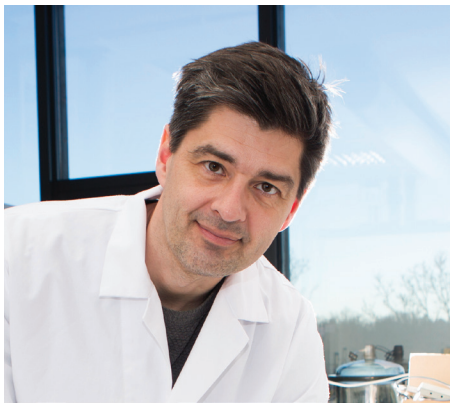
At the University of Cape Town, Nicolas von Solms was selected as the Visiting Engineering Professional by the department of chemical engineering, and he gave a research seminar in this capacity.
At University of Stellenbosch he also gave a seminar and further attended a conference celebrating the 50-year anniversary of the chemical engineering department.

Summer Course Tradition Stands Strong

For more than 20 years has CERE hosted a summer course on thermodynamic models for its own PhDs and industry, the "Advanced Course on Thermodynamic Models: Fundamentals & Computational Aspects".

Originally initiated by Professors Michael L. Michelsen and Jørgen Mollerup, since 2015 the course has been organized by Professor Georgios Kontogeorgis and Associate Professor Wei Yan. The 2019 version of the course attracted a record number of international participants, 21 from nine countries. Once again, the course was evaluated very positively by the participants, and CERE will continue the tradition in coming years.

Invited to inspire Future Innovators



Senior Researcher Nikolaj Sorgenfrei Blom

Senior Researcher Nikolaj Sorgenfrei Blom, CERE, was invited as key note speaker at the Founders of Tomorrow impact bootcamp held in Copenhagen, 24 February – 1 March. Founders of Tomorrow is a non-profit educational bootcamp and idea competition. During the event, 60 selected participants are gathered to learn about purpose-driven innovation and use of technology to create a positive impact in the world.

In his presentation, Nikolaj Sorgenfrei Blom explained his area of research within electromagnetic fields, DNA and new properties of water. He further addressed how this emerging field – known as quantum biology or bio-resonance – is challenging traditional views and may lead to scientific disruption.

Founders of Tomorrow (formerly Danske iDeer) is an annual event funded by the Danish Industry's Foundation.

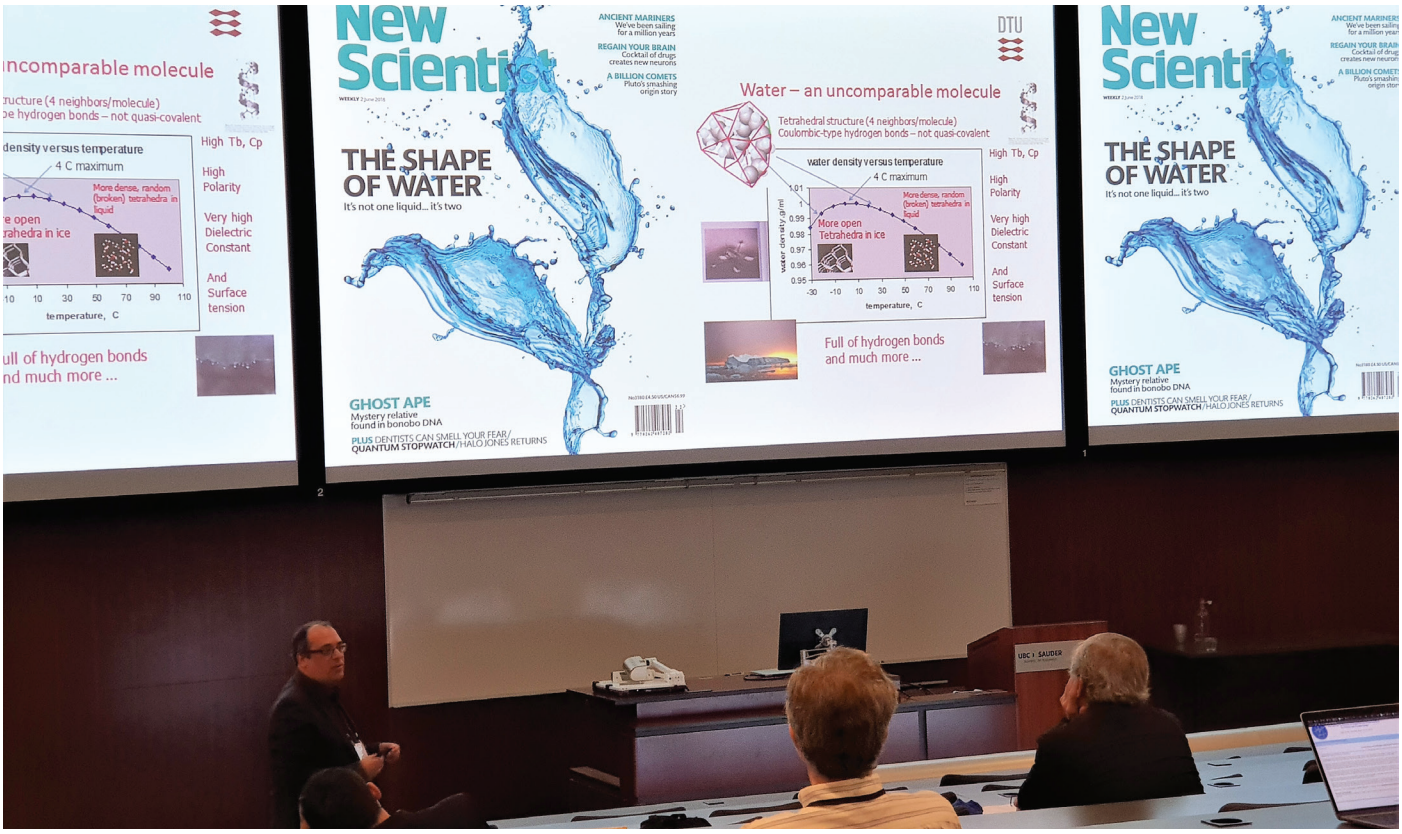
Visiting Professor in Xining, China

Associate Professor Kaj Thomsen

Associate Professor Kaj Thomsen has been appointed as a visiting professor of Qinghai Institute of Salt Lakes, Chinese Academy of Sciences. The engagement is for a period of four years (Sep. 1, 2019 – Aug. 31, 2023).

Following the retirement from DTU at the end of June, 2020, Kaj Thomsen is expected to teach courses on electrolyte solution thermodynamics at QISLCAS, Xining, China.

Presence at International Chemical Engineering Events



From Kanazawa to Florence, CERE researchers were present at scientific conferences in chemical engineering throughout 2019. Among the major participations of the year were:

PPEPPD

The Properties and Phase Equilibria for Product and Process Design (PPEPPD) conference in Vancouver, Canada, 12-16 May, was attended by Professor Georgios Kontogeorgis, Associate Professor Xiaodong Liang, and PhD students Edgar Luis Camacho Vergara and Spardha Virendra Jhamb.

Professor Kontogeorgis gave an oral presentation on electrolyte thermodynamics, while Xiaodong Liang, Edgar Luis Camacho Vergara and Spardha Virendra Jhamb presented a total of five posters within the topics of density gradient theory, PT Flash, and computer-aided product design.

Petrophase

The Petrophase conference in Kanazawa, Japan, 1-6 June, was attended by Associate Professor Nicolas von Solms. One of his core interests is recovery of methane from natural gas hydrates. For the first time, the Petrophase conference had a dedicated session on this topic. Petrophase is the premier academic conference dedicated to the petroleum chemistry, phase behaviour and flow assurance.

TCCS

A nine people strong delegation from CERE attended TCCS 10 - the 10th Trondheim conference on CO2 Capture, Transport and Storage (CCS), 17-19 June. The Norwegian conference is a bi-annual event which has become globally leading within CCS.

The CERE participants were Associate Professor Philip L. Fosbøl, Postdocs Humbul Suleman and Susana Almeida, Research Assistant Randi Neerup, PhD students Lucas Farias Falcchi Corrêa and Sebastian Nis Bay Villadsen, and MSc students Ameya Sunil Joshi, Jens Kristian Jørsboe and Sai Hema Bhavya Vinjarapu.

SCA

The 33rd International Symposium of the Society of Core Analysts (SCA) was held in Pau, France, 26-30 August. PhD student Jyoti Shanker Pandey presented his poster on Methane Production from Gas Hydrate Deposits in Sandy Porous Media under Permafrost Temperature Conditions. SCA is a chapter of the Society of Petro-physicists and Well Log Analysts (SPWLA).

EECE 12

Last but not least, the 12th European Congress of Chemical Engineering (EECE 12) was held in Florence, Italy, 15-19 September. With more than 1,300 participants from Europe, Asia and America, EECE 12 was the biggest European event for chemical engineers from both industry and academia. Three CERE researchers attended.

Postdoc Olivia Ana Perederic gave an overview presentation on Systematic Computer-aided Methods and Tools for Lipid Process Technology. PhD student Yiqun Liu disseminated his work on Phase Equilibrium and Density of Highly Asymmetric Gas-Oil Mixtures at High Temperatures and High Pressures. And finally, PhD student Xinyan Liu presented a poster on Ionic Liquid Design and Process Simulation for Shale Gas Separation.

Hosting Society of Petroleum Engineers Event

On 22 November 2019, DTU hosted a meeting of the Copenhagen section of the Society of Petroleum Engineers (SPE). The event was organized jointly by the Danish Hydrocarbon Research and Technology Centre, (DHRTC) and CERE.

SPE is active worldwide, organizing a number of conferences and workshops every month and publishing several journals on engineering research. The Copenhagen SPE section involves representatives of all the most important petroleum companies operating in Denmark. At DTU a Student Chapter is active, at present amounting to ca. 8 members. Collaboration between the Student Chapter and the "adult" SPE makes it possible to establish regular contacts between the students and the professionals, which is very important for the students' professional development and, eventually, for their future employment.

The SPE Copenhagen section, among other activities, organizes monthly SPE meetings. These meetings are being organized by the petroleum companies, at different places around Copenhagen. Once a year, a meeting is traditionally hosted by DTU. This is the way for the DTU researchers to present their recent results to the industry. This year the meeting was especially well attended with around 100 participants from academia and industry.

Keynote speakers were Director Morten Jeppesen, DHRTC, and Professor John Bagterp Jørgensen (CERE, DTU Compute). Morten Jeppesen presented his views on the future Danish oil and gas production and the role of DHRTC, while John Bagterp Jørgensen talked about perspectives in digitalization and optimization of the upstream oil and gas industry.

The presentations were followed by dinner, during which Researcher Ali Eftekhari, DHRTC, gave an entertaining talk about the balance between sustainable and traditional sources of energy in Denmark.

Director Morten Jeppesen, DHRTC.

Professor John Bagterp Jørgensen, CERE.

President of SPE Student Chapter DTU Hadise Baghooee.

Researcher Ali Eftekhari, DHRTC.

New project with Petrochina

Associate Professor Xiaodong Liang (PI) and Professor Georgios M. Kontogeorgis have received a project funded from PetroChina, which supports fundamental research on water structure and hydrogen bonding behaviour with molecular simulations, theories and models. One PhD student and one Postdoc will be employed in this project. The Postdoc has started while the PhD is expected to start in early 2020.

Project on the Heartbeat of Life

Beating 7.83 times per second, the Earth has a pulse of its own. Known as the Schumann resonance, this very weak electromagnetic field is caused by atmospheric lightning in the Earth-ionosphere cavity. Presumably, this "heartbeat" has been present since the beginning of life on our planet, and a new project headed by Senior Researcher Nikolaj Sorgenfrei Blom, CERE, will investigate whether health at the cellular level is affected by geomagnetic fields such as the Schumann resonance field.
The project, GeoHealth, is sponsored by the Lundbeck Foundation Experiment Grant with 2 million DKK. The project will be performed in collaboration with stem cell researchers at DTU Bioengineering. The project is to commence in spring 2020 with a two-year duration.

Article selected for Golden Open Access

Professor Georgios Kontogeorgis

The article "Taking Another Look at the van der Waals Equation of State – Almost 150 Years Later", co-written by Professor Georgios Kontogeorgis, CERE, with French professors Romain Privat and Jean-Noël Jaubert, has been selected as a Golden Open Access article by ACS (American Chemical Socieity) journals' editors, thus available free to anyone interested.
https://pubs.acs.org/doi/10.1021/acs.jced.9b00264

Work of PhD Student highly praised

Dr. Duncan Paterson has been granted a Springer Thesis Award for his PhD thesis on Flash Computation and EoS Modelling for Compositional Thermal Simulation of Flow in Porous Media.

Duncan Paterson

Besides Euro 500, the award involves publication of the work in Springer's collection of outstanding dissertations "Springer Theses". The Springer Theses are selected from internationally top-ranked research institutes. Over the past six years, the program has helped disseminate the contributions of over 500 talented young scientists. Many of them have gone on to win other awards and /or take up leading research positions. Dr. Paterson graduated in 2017 with supervisors Associate Professor Wei Yan, Professor Michael L. Michelsen, and Professor Erling H. Stenby. He is currently at Linde.

In addition, Duncan's PhD was nominated for the EFCE (European Federation of Chemical Engineering) Excellence Award in Thermodynamics and Transport Properties 2019 and was ranked as the second- best thesis in the competition: "the Award jury gave special recognition to the runner-up, Dr. Duncan Paterson, Denmark, for his excellent PhD thesis "Flash Computation and EoS Modelling for Compositional Thermal Simulation of Flow in Porous Media" for which he achieved the second-best evaluation results. The research originates from the need for describing the complex process of recovering heavy oil with steam and solvents for the sake of reducing the energy and water consumption and the associated CO2 emission. During his thesis, he has given unique contributions in generic algorithms for multiphase flash, and in particular the RAND-based flash framework which allows simultaneous computation of chemical equilibrium. It is expected that the formulations developed in his thesis will have a long-lasting impact on how we perform multiphase flash calculation under various specifications, with or without chemical equilibrium."

Biogas electro-scrubbing goes full-scale

Sulphur and other impurities in biogas reduce the commercial value of the gas, and may also hamper upgrading into higher-value chemicals. Electro-scrubbing, a technology developed by CERE and partners, promises to be better than current state-of-the-art methods for removal of impurities from biogas.

Funded by a grant from the EUDP technology program of the Danish Energy Board, CERE and industry partners Elplatek, Union Engineering and DGC aim to develop a first-of-a-kind full-scale demonstration plant based on electro-scrubbing. The project is named BE-Clean.

The technology has been developed in a recent project, MeGa-StoRE, which was mainly focussed on conversion of biogas into methane. As the importance of biogas purification became apparent in that project, the interest in investigating electro-scrubbing arose. While the technology has been developed for desulfurization by the partners, removal of several other types of impurities will also be looked at in the new project.

The BE-Clean project is coordinated by Associate Professor Philip L. Fosbøl, CERE, and will have a duration of three years.

Biogas-to-methanol demonstration unit

Conversion into methanol will greatly increase the value of biogas. Following 2.5 years of successful lab-scale tests, CERE and partners have been granted support for construction and test of a biogas-to-methanol demonstration unit.

Today, biogas is either converted to electricity/heat or upgraded to methane. Methanol has a higher value than both of these solutions.

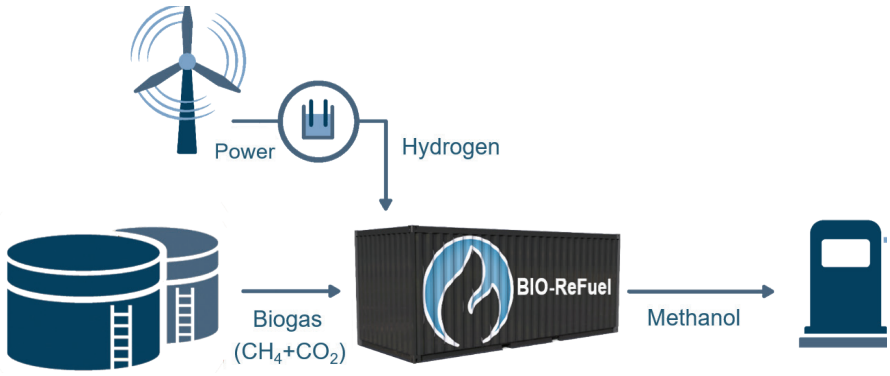
According to estimates, up to 50 % of the energy demand for transport in Denmark can be covered by methanol from biogas.
In the project BIO-ReFuel (phase 1), CERE and industry partners Elplatek, Unicat Catalyst Technologies, and Lemvig Biogas have developed a novel catalytic technology.

The technology has been successfully tested and fine-tuned in lab-scale. The same partners, with the addition of new industry partner Union Engineering (part of Pentair), are ready to take the technology into phase 2. Both phases have been granted support from the Danish Energy Board under its technology demonstration program EUDP.

The main focus of phase 2 will be the construction and testing of a demonstration unit. The unit will be fitted into a standard, ISO-size container. This is to allow for easy transportation as the technology will hopefully be purchased by biogas producers across Denmark and abroad.

The demonstration unit will be dimensioned for processing of 240 m3 of biogas per day. The process may run either with or without addition of hydrogen. If hydrogen is added, extra methanol can be produced.

BIO-ReFuel (phase 2) is coordinated by Associate Professor Philip L. Fosbøl, CERE. The project will run for three years.



Synergy with KT-Consortium

The synergy between CERE and KT-Consortium has grown strong during 2019, including the Discussion Meetings of the two Consortia held once again in June in the same period and at the same venue with one joint day. More synergy aspects are:

Participation at DTU High Tech Summit

PhD Student Spardha Virendra Jhamb and Associate Professor Xiaodong Liang represented DTU Chemical Engineering at the DTU High Tech Summit 2019.

Xiaodong gave a talk on Computer-aided tools in Sustainable Product Design, including case studies on hazardous chemicals, solvent selection for coatings formulations and developing a model for the prediction of biodegradation of organic compounds. This was followed by a demonstration of the ICAS software developed at KT Consortium by Spardha, who demonstrated two out of the many tools available in this software, namely ProCAMD for the design of organic compounds and mixtures using group-contribution property models and VPPD-Lab for chemical formulation design.

Discussions following the demonstration raised keen interest in the capabilities of the software. The participation in this event is foreseen to open doors for collaboration across various departments at DTU.

EU H2020 Project RENESENG II

Postdoc Olivia Ana Perederic

Renewable Systems Engineering for Waste Valorization II (RENESENG II) is a project under the HORIZON 2020 program, which DTU joined in May 2019.

The project has seven academic and six industry partners (based in Europe, USA and Australia), one being Arkema (member of KT-Consortium).

The project is coordinated by Professors John M. Woodley and Georgios M. Kontogeorgis.

Within the project, Dr. Olivia A. Perederic started a secondment with Arkema and will work on a project regarding the synthesis of an economically viable process for fatty dicarboxylic acids production

(www.reneseng2.com/).

The project goal is to further advance the emerging area of Bio-Process Systems Engineering by capitalizing the advances in the previous RENESENG project, where DTU was also a partner.

New Project on Predicting Biodegradability

The project Developing a Group Contribution Model (GC) for Biodegradation-related Properties, started on 28 January 2019, and was conducted by visiting MSc student, Irene Hospital and supervised (at DTU) by Professor Georgios M. Kontogeorgis, Associate Professor Xiaodong Liang and PhD Student Spardha V. Jhamb.

The project proposal was given by Syngenta AG, and DTU is continuing to collaborate with the company on several aspects of the project.

The study of biodegradation of chemicals that are discharged into the water bodies is important to determine the risk to the environment that is associated with the chemical.

Hence, there is a requirement for measurement and systematic consolidation of data on biodegradation in order to assess the persistence of a chemical in the environment.

Considering the criteria given by European Chemical Agency (EChA) to classify a chemical as 'persistent in the environment', the potential for the development of a group-contribution (GC) model has been recognised.

This model would be useful when experimental data on biodegradation for an organic compound is not available.

The final goal of the project is to have a biodegradability prediction model in the ProPred and ProCAMD tools of the ICAS Software.

New Software Manager

Software manager Guoliang Wang

As of 15 October 2019, Dr. Guoliang Wang has been employed as the new Software Manager of the KT Consortium and the CERE Consortia (following Edgar Vergara and Dr. Alay Arya who held these positions previously).

Cubic EoS: New Math to the Rescue

Jean - Noël Jaubert, Professor of Chem. Engineering at the Université de Lorraine

Cubic Equations-of-State (EoS) are widely applied for modelling fluid thermodynamic properties in oil and gas processing and numerous other chemical engineering applications.

The use of cubic EoS relies on a temperature-dependent parameter, the alpha function. Jean -Noël Jaubert, Professor of Chemical Engineering Thermodynamics at the Université de Lorraine, France, presented new mathematical tools for application of alpha functions in EoS.

"Our recent investigations have made it possible to conclude that to get accurate and physically meaningful behaviours in both the subcritical and supercritical domains, it is necessary to work with a consistent alpha function, i.e., with an alpha function which is positive, decreasing and with a negative third derivative," Professor Jaubert stated.

"Mathematical constraints that imperatively need to be applied to α-function of cubic EoS to get accurate and physically sound results." 21 January.

No Time like the Present

Andrew Holster, Massey University

The concept of reversibility is important in both particle physics and in chemistry and statistical thermodynamics treating larger aggregate systems.

This concept – also known as time reversal symmetry – stems from the assumption, that fundamental quantum mechanical processes can be reversed.

Dr. Andrew Holster, of Massey University, New Zealand, presented a new view on the subject.
"We are often told that processes are time reversible at a fundamental level. But even simple processes in chemistry are entirely irreversible in practice (...). The principle of micro-reversibility as normally defined in physics does not represent time reversal as commonly assumed, but instead represents a combination of time reversal and causal exchange," according to Dr. Holster.
"It corresponds to time reversibility only for equilibrium systems, when the principle of detailed balance also holds. But most real-world problems, including chemical processes, are strongly irreversible."

"Reversibility of probabilistic processes in physics and chemistry." 3 May.

Energy-efficient Desalination of Water

André J. Burger of University of Stellenbosch

As many countries suffer from water scarcity, interest in desalination of sea water is high. Membrane desalination is a mature technology, but its wider implementation is slowed down by various challenges, mainly relatively high costs.

Solutions to these challenges were addressed by Professor André J. Burger of University of Stellenbosch, South Africa. "Today, large plants are successfully operated world-wide (...). However, while those who are intimately involved with the operation of such plants are perhaps mostly focusing on the minimization of membrane fouling and cleaning, one of the more popular public criticisms against desalination is that it is energy intensive, expensive and unsustainable.

This is not unfounded criticism if one considers, for example, that the power consumption of a sea water reverse osmosis plant contributes to more than 50 % of operating costs," said Professor Burger.

He went on to explain several aspects of power consumption during membrane desalination, focusing on theoretical minimum energy requirements, energy efficient configurations and energy recovery methods.

"Membrane desalination: concepts and perspectives related to thermodynamics and energy consumption." 7 June.

Storage of Natural Gas as Hydrates

Gaurav Bhattacharjee, the National University of Singapore

Solidified Natural Gas (SNG) technology has emerged as an alternative concept for natural gas storage.

With an ongoing flagship project, Singapore is leading in the field. Dr. Gaurav Bhattacharjee, Senior Research Fellow with the National University of Singapore, showcased experience in both various applications of gas hydrates and in the recovery of natural gas from marine gas hydrate reservoirs.

"SNG technology has gained popularity owing to its environmentally benign operation, large volumetric capacity and non-explosive character (...). Our group has been able to not only favourably tune the thermodynamic operating conditions for hydrate formation – so, significantly higher temperature and lower pressure for hydrate formation – but also demonstrated remarkable kinetic performance during hydrate formation at the revised operating conditions," noted Dr. Bhattacharjee.

He went on to inform the audience on customized experimental facilities for the purpose, and explain a roadmap developed for the further expansion of the technology.

"The Case for Solidified Natural Gas (SNG) Technology." 20 August.

Quantum Effects behind the Water Bridge

Application of high voltage to two neighbouring open water containers is able to create a bridge of floating water between them. This is just one of several yet-to-be-understood phenomena relating to water, according to Adam Wexler, Chief Scientist at Joi Scientific, Inc.

"Liquid matter represents a challenge to our current notions of how matter and energy organize (...). Recent work on a class of non-equilibrium phenomena where liquids develop unusual and easily observable behaviour, such as flowing between two containers under the influence of an electric field, have revealed that not only are there non-trivial interactions at intermediate length scales, but that there are demonstrable changes in the organization of such systems that indicate the onset of quantum control on continuum properties," said Adam Wexler.

The main activity of Joi Scientific, headquartered at the Kennedy Space Center Life Sciences Lab, USA, is extraction technology to produce hydrogen gas from water. In his talk, Adam Wexler presented both theoretical considerations and experimental observations on the dynamics and structure of water.

"Can an electrically induced phase transition occur in room temperature liquid water?" 8 October.

Modelling of strong Electrolyte Solutions

Darren Rowland, the University of Western Australia

Pitzer equations have been widely adopted as a thermodynamic modelling framework for aqueous electrolyte solutions. This is due in part to the simplicity with which diverse thermodynamic properties can be correlated in a single model. Dr. Darren Rowland, Postdoc at the University of Western Australia, offered his views on the subject. "A key strength of the Pitzer equations is their flexibility to cover broad ranges of pressure and/or temperature.

However, due to the lack of a strong theoretical foundation, the number of adjustable parameters required - and number of data required to regress those parameters – can be worryingly large (...). Although fits can be achieved (...) these fits tend to be unsatisfactory if the data have gaps and other deficiencies.

Too frequently, the flexibility of the Pitzer equations manifests in violations of known thermodynamic behaviour," Darren Rowland noted, continuing to outline strategies for overcoming some of the limitations for the Pitzer equations.

"Approaches for Developing Thermodynamic Equations of State for Strong Electrolytes Based on the Pitzer Equations." 6 November.

Activity of Individual Ions in Aqueous Solutions

Juan H. Vera, McGill University

For more than eighty years, measuring the activity of individual ions in aqueous solutions was believed to be impossible. This was the commonly accepted paradigm. However, a few researchers were brave enough to publish electrochemical measurements from which such activities could be obtained.
Professors Grazyna Wilczek and Juan H. Vera, McGill University, figured out that there were commercial ion selective electrodes to measure the mean ionic activity coefficients of electrolytes in aqueous solutions, and reasoned that from the response of the ion selective electrode of each of the two individual ions of a salt, information could be obtained on the activity of the individual ion.

As many well-established researchers were against this concept, this was a difficult path. All the work done measuring the activities of individual ions was done either with postdoctoral students or visiting scientists. In their talk, Wilczek and Vera presented the story of a difficult path on a changing paradigm.

"The Activity of the Individual Ions in Aqueous Solutions. Are they Real or Imaginary?" 12 December.

Natural Gas Processing at the Sea Floor

Francois Johan Kruger, PhD
Currently with BASF, Ludwigshafen, Germany.
Full title: "Towards the Realization of Subsea Factories: Thermodynamics of Petroleum Fluids relevant to Subsea Processing."
Supervisors: Nicolas von Solms, Georgios Kontogeorgis.
Funded by: Equinor.

In 2015, Equinor commissioned the world's first subsea compressors, at the Åsgard subsea facility at depth 300 meter underlining the company's status as a leader in subsea processing. Treating freshly produced natural gas already at the seabed offers a number of advantages over traditional treatment at offshore platforms or onshore facilities. Substantial amounts of energy and chemicals can be saved, and operators will be able to access resources further away from their base facilities. The project, which was conducted in collaboration with Equinor, contributes to development of subsea processing.

Traditional treatment of gas at an offshore platform or at onshore facilities involves wasting considerable amounts of energy for transporting multiphase streams. By instead conducting the processing at the seabed, one can take advantage of the high pressure which is often thermodynamically beneficial. And even more importantly, single-phase transport lines can be installed. This means that the pressure drop across pipelines decreases significantly and phenomena such as slugging are avoided. Much longer pipelines can be installed – i.e. tie-back distances are increased – without the need for intermediate platforms or boosting, and therefore more remote resources can be effectively recovered.

Subsea processing may also significantly decrease the amounts of chemicals needed for gas hydrate inhibition. At Åsgaard, subsea compressors are already used to boost gas production, and at Gulfaks a smaller wet gas compressor is in operation. Compressors not only increase production but also extend the reservoir lifetime by effectively producing additional gas.

At CERE's laboratories in Denmark, an experimental apparatus was modified for the quantification of C1-nC6/nC7-H2O phase distributions (VLLE) at 303-323 K. Good agreement was achieved with several binary VLE sources from literature.

Two-phase data directly relevant to the natural gas dehydration step were measured during an external research stay at Equinor in Norway. C1-MEG-H2O and (natural) gas-MEG-H2O systems were investigated for temperatures in the range 288-323 K and pressures of 60 and 125 bar. In modelling of the ternary data, CPA (Cubic Plus Association) was found to provide superior prediction over the SRK-HV equation of state.

New ways of accounting for the hydrogen bonding in MEG were proposed, and the importance of using raw experimental data in parameter regression was highlighted. Overall results showed that no scheme is universally superior, but improved prediction over the literature parameters was achieved in all cases, including in the prediction of ternary data.

Combined parameter uncertainty and process input sensitivity analyses were performed for simplified natural gas dehydration configurations. Using Monte Carlo simulation, distributions were generated for process outputs such as a product gas quality. Process conditions were optimized to achieve the desired specifications with a 99.7 % confidence interval.

An illustration of The Subsea Factory TM – Equinor

CO_2 as a Valuable Raw Material

Xianglei Meng, PhD
Currently with the Institute of Process Engineering, Beijing, China.
Full title: "Conversion of CO_2 to Carbonates Catalyzed by Ionic Liquids under Mild Conditions."
Supervisors: Nicolas von Solms, Suojiang Zhang.
Funded by: DTU Chemical Engineering and Institute of Process Engineering, Chinese Academy of Sciences.

The global warming crisis has increased interest in using CO_2 as a raw material rather than emitting this greenhouse gas into the atmosphere. However, as CO_2 is the highest oxidation state of C, activation of CO_2 requires energy input. Hence only a small number of chemical pathways for utilization exist. In the project, several new catalytic routes have been developed.

A feasible utilization of CO_2 is as a raw material for synthesis of five-membered cyclic carbonates. This can be achieved by cyclo-addition of CO_2 with epoxides, which is one of the few industrially successful processes which utilize CO_2. Cyclic carbonate is widely used as solvent in chemical processes, electrolyte components in lithium batteries, monomers for acyclic carbamates, and several other applications.

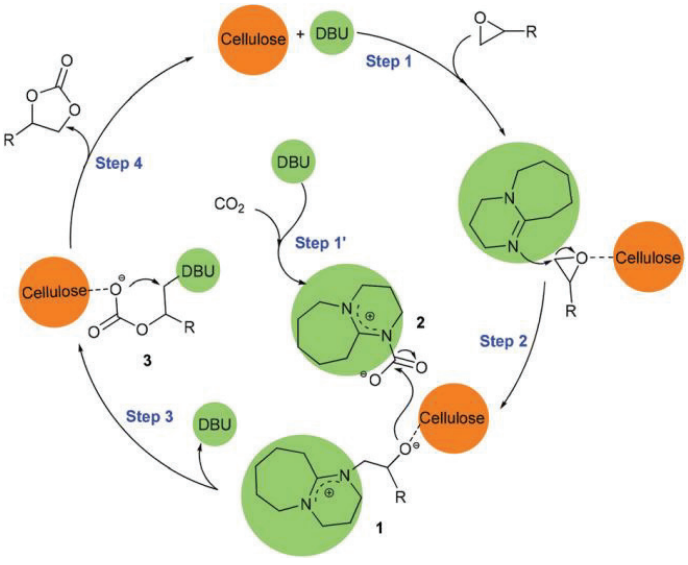
The focus of the project is carbonate synthesis based on functional ionic liquids (ILs) catalysis. ILs are liquid organic salts, entirely composed of organic cations and organic/inorganic anions at or near room temperature. ILs have a number of desirable properties making them attractive as environmentally benign solvents.

Firstly, 1,8-diazabicyclo-[5.4.0]undec-7-ene (DBU) based bi-functional protic ionic liquids (DBPILs) were prepared by acid-base reaction. The best DBPILs showed a 92 % yield of products within 6 hours at 30 °C and 1 bar CO_2 without any solvents or co-catalysts. Carbonates were afforded in good yields with CO_2 from simulated flue gas (15%CO2/85%N2). The DBPILs were able to activate both CO_2 and epoxide by the alkoxy anion and powerful hydrogen bonding.

Secondly, DBU based ILs containing Al (DILA) catalysts were synthesized. DILA was used as a single-component and solvent-free catalyst for the conversion of CO_2 to cyclic carbonates with epoxide at mild conditions. DILA showed a catalytic activity of 94 % within 6 hours at 30 °C and 1 bar CO_2. Furthermore, DILA was found suitable for a broad epoxide substrate scope and could be easily recycled at least four times without obvious loss of activity.

Thirdly, a series of cross-linked poly(vinylimidazole/butyl acrylate) ionic liquids membranes (PVBILs) were prepared and used as efficient heterogeneous catalysts for fixation of CO_2 with epoxide at mild conditions. The best PVBILs showed a 90 % yield of carbonate within 24 hours at 50 °C and 1 bar of CO_2.

Finally, a series of metallo-porphyrin ILs (MPILs) were designed and synthesized by a one-step method. The MPILs combine the advantages of IL and porphyrin. These catalysts have multiple active sites and a good capacity for visible light absorption, which is highly beneficial as the absorption of light adds energy to the process, greatly lowering the need for other energy inputs. The MPILs were successfully used as photocatalysts in cyclo-addition of CO_2 with epoxide to produce carbonate at room temperature and 1 bar pressure under irradiation of visible light.



The mechanism for the DBU-cellulose catalysed reaction.

Electrolyte Modelling with e-CPA

Li Sun, PhD
Currently Research Assistant at CERE
Full title: "Analysis and Applications of the Electrolyte Cubic-Plus-Association Equation of State".
Supervisors: Georgios Kontogeorgis, Xiaodong Liang, Nicolas von Solms.
The project was supported by DTU Chemical Engineering and by China Scholarship Council.

Electrolyte solutions find numerous applications in physical sciences including chemistry, geology, material science, medicine, biochemistry and physiology as well as in many engineering fields especially chemical, biochemical, electrical, petroleum and environmental engineering.

Thermodynamics is crucial for industry applications. When electrolytes (salts or some ionic compounds) are dissolved, they dissociate into ions that have lost or gained electrons. As an implication, three different types of interactions will be present in the solution: molecule-molecule, ion-ion, and molecule-ion. This complexity introduces additional challenges in thermodynamic modelling.

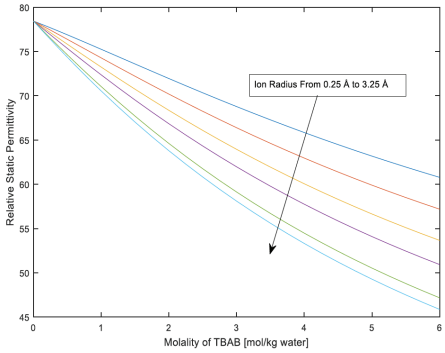
In the project, the use of the electrolyte Cubic Plus Association Equation of State (e-CPA EoS), an extension of the CPA EoS with the Dybye-Hückel theory for the ion-ion electrostatic interactions and the Born term for ion solvation added, for electrolyte solution modelling is investigated with a special attention on gas hydrate related systems. Gas hydrates are substances resembling snow or ice. Under certain conditions they may precipitate in production gear during oil and gas production, potentially causing significant economic losses. Gas hydrates also have considerable potential as storage and separation media for various gases. Both promotion and inhibition are therefore of interest, and thermodynamic studies are equally important in either context.

In the first part of the project, thermodynamic modelling of aqueous solutions of both quaternary ammonium salts (QAS) and metal halide salts was done. For QAS systems (single salt systems), the results show that eCPA can satisfactorily correlate the mean ionic activity coefficients and the osmotic coefficients.For metal halide salt systems (systems with multiple salts), the adjustable model parameters of single salt systems were used for direct modelling.

The results show that eCPA can predict the mean ionic activity coefficients of aqueous multi-salt solutions well by using single-salt interaction parameters.

In the second part of the project, gas solubilities in aqueous electrolyte solutions were modelled. The adjustable parameters were obtained by fitting the experimental data of gas solubilities in single-salt solutions. The results show that the model can satisfactorily correlate gas solubilities over a wide range of conditions for most systems. Further, the model was applied for prediction of gas solubility in multi-salt solutions, also with a satisfactory performance.

Finally, a modelling study was carried out for individual ion activities in aqueous electrolyte solutions with e-CPA EoS and other approaches.



Predicted relative static permittivity of the aqueous Tetra-n-butyl Ammonium Bromide solution at 298.15 K using the e-CPA EOS

Modelling of Electrolyte Solutions

Anders Tviis Schlaikjer, PhD.
Currently with Novo Nordisk Pharmatech
Full title: "Development of the Electrolyte CPA Equation of State".
Supervisors: Georgios Kontogeorgis, Kaj Thomsen.
The project was funded by the joint industry project Chemicals in Gas Processing (CHIGP) and DTU Chemical Engineering

Solutions containing electrolytes are important in many chemical processes. Examples are energy storage in batteries, acid gas cleaning, carbon capture, and production of fertilizers. Presence of electrolytes can change the behaviour of solutions, for instance by introducing phase separation in otherwise miscible solutions. This is a well-known problem in the petroleum industry, where the presence of electrolytes can cause scaling in production gear. Modelling of electrolyte solutions is therefore highly relevant.

Focus of the project is the eCPA EoS (electrolyte Cubic Plus Association Equation of State).

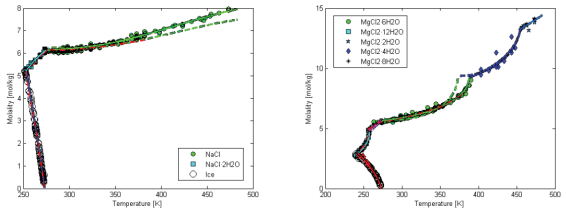
In the first section of the project, the eCPA EoS was parametrized in a salt-specific framework for 12 salts using salt solubility data as well as osmotic coefficient and mean ionic activity coefficient data. The inclusion of solubility data was seen to only affect the average deviations of osmotic coefficients and activity coefficients slightly. The increase was almost entirely due to reduced accuracy at high temperatures and high molality.

Furthermore, the model was compared to the activity coefficient model Extended UNIQUAC. It was shown that eCPA provides more accurate solubility description at higher temperatures than Extended UNIQUAC, while the later model is slightly better at describing the activity coefficients. Overall, the two models perform similarly.

Using a salt-specific framework, as in the first section of the project, does imply certain limitations. A such framework can only be applied when a common ion is found between the salts in the solution. Therefore, an optimization routine for obtaining ion-specific parameters was developed in the second part of the project. Ion-specific parameters were estimated by a simultaneous fitting of parameters for 17 ions, consisting of ten cations and seven anions, and with data for 55 salts.

The parameters were fitted to the osmotic coefficient and mean ionic activity coefficient data in a wide temperature range from 273.15 K to above 500 K and up to an ionic strength of 6 molal. It was found that use of ion-specific parameters in some cases requires inclusion of adjustable parameters. The parameter set were found to yield similar deviations as the salt-specific parameters. However, a few salts cation-anion interaction parameters were needed to obtain reasonable accuracy.

Finally, the ion-specific parameters were applied to a series of systems, which included mixed salt osmotic coefficients, solid-liquid equilibrium, and vapour-liquid equilibrium of water-methanol-salt. Modelling of mixed salt osmotic coefficients illustrate that the parameters work well in salt mixtures, while the phase equilibria also illustrate the extension to mixed solvent systems.



(a) NaCl (b) $MgCl_2$

Freezing point and solubility as a function of temperature, on the left for a NaCl solution, on the right for a MgCl2 solution

Enhancing Production of Major Oil Fields

Lasse Hjuler Christensen, PhD

Currently Software Developer at SimCorp
Full title: "Optimal Control of PDE-constrained Systems".
Supervisors: John Bagterp Jørgensen, Allan Peter Engsig-Karup, Michael Pedersen.
Funded by: the OPTION project.

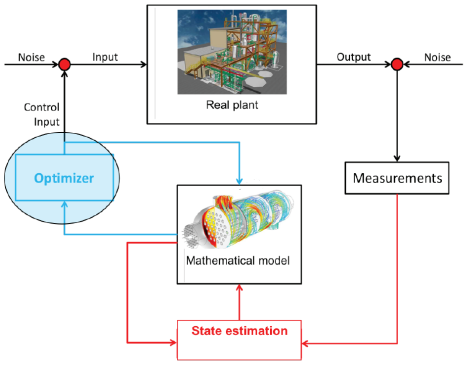
Nonlinear model predictive control (NMPC) is a promising methodology for enhancing the production of major offshore oil fields. In this context, NMPC will take the form of closed-loop reservoir management (CLRM) with the goal of determining the optimal operating profile which maximizes economic performance over the reservoir life-cycle. The project presents new computational methodologies that contribute to fast, memory-efficient and robust CLRM solutions.

Oil production often involves multiple injection and production wells across the same oilfield, and the interaction between these wells can be complex. Thus, the chosen production strategy will have a significant impact on the profitability over the total life time of the field. To manually devise the optimal strategy is non-trivial and time-consuming. While CLRM has emerged as a promising alternative, real-life application is challenged by geological and economic uncertainties.

In the first part of the project, new methodologies for addressing the risks involved by using uncertain and possibly even errant model data have been developed. Conventional risk mitigation strategies typically rely on multi-query solution of large-scale optimization problems constrained by partial differential equations (PDEs). As a consequence, conventional methods often become computationally intractable in practice. Instead, the proposed strategies seek to address uncertainty using approaches based on PDE-constrained multi-objective optimization. A selection of numerical case studies demonstrates proof-of-concept: the new risk mitigation strategies pose a computationally attractive and scalable alternative to conventional methods.

The second part of the project was devoted to development of customized iterative solvers for time-dependent PDE-constrained optimization problems governed by systems of non-linear diffusion-reaction (DR) equations. The solvers are based on a new high-order approach combining spectral discretization schemes with appropriate Krylov subspace (KSP) methods. The solvers specifically target distributed control problems in separable domains; examples include control of the Schlögl model, Fitz-Hugh-Nagumo problems and coupled systems of DR equations which govern chemical reactions. The solvers allow for both subdomain control and additional point-wise bound constraints.

As a key feature, the high-order approach introduces a new type of Poisson-like preconditioners that are tailored for efficient solution of the large-scale saddle-point problems that constitute the computational bottleneck of Newton-like optimization algorithms such as Sequential Quadratic Programming methods. By construction, the preconditioners are matrix-free, scalable with respect to the spatial problem dimension, and prone to parallelization. Numerical studies indicate that the preconditioners are ideal for more complex cases of non-linear and time-dependent DR problems. Further, the results show that the new iterative solvers outperform state-of-the-art direct methods and may pose viable alternatives to the widely used constellation of low-order schemes and Schur-complement block preconditioners.

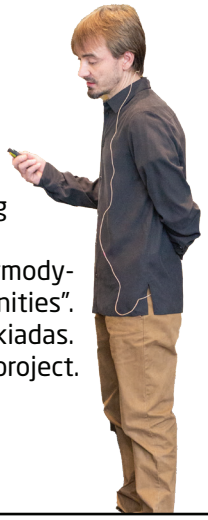


Conceptual illustration the key constituents of NMPC

Syngas Fermentation to Biofuels

Antonio Grimalt-Alemany, PhD
Currently Postdoc at DTU Chemical Engineering

Full title: "Syngas Fermentation to Biofuels: Evaluation of the Interplay of Kinetics and Thermodynamics for Directing Bioconversions based on Mixed Microbial Communities".
Supervisors: Hariklia Gavala, Ioannis Skiadas.
Funded by the SYNFERON project.



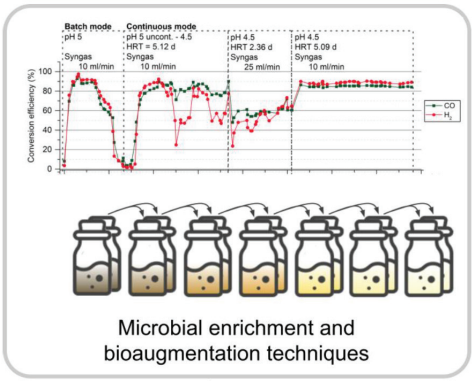
Microbial systems are expected to play an important role in sustainable production of commodity chemicals, biofuels and biomaterials. The use of microbial communities is currently expanding from conventional anaerobic digestion towards innovative platforms. The project investigates one such platform, namely fermentation of syngas for the synthesis of valuable products with low operating costs.

Several types of biomass can be converted through gasification into syngas, which is a mixture of mainly H2, CO, and CO2. Through fermentation under anaerobic conditions it is possible to convert syngas further into a range of products including CH4 (methane), H2 (hydrogen), carboxylic acids (acetate, butyrate and caproate), and solvents (ethanol, butanol, and hexanol).

From a practical viewpoint, microbial communities have several benefits over using single microbial species, mainly high resilience to process disturbances, the possibility of stable operation in continuous mode under non-sterile conditions, and low costs of operation. Nevertheless, they also constitute a limitation, as the poor understanding of their complex network of metabolic interactions often results in limited control of their metabolism, ultimately hindering the control of the process and their product selectivity. Thus, the project evaluates the potential of several microbial community management strategies including directing the natural selection of microorganisms through microbial enrichments, the use of thermodynamic principles for designing operational strategies, and the use of modelling tools for ultimately improving the control over the activity of microbial communities.

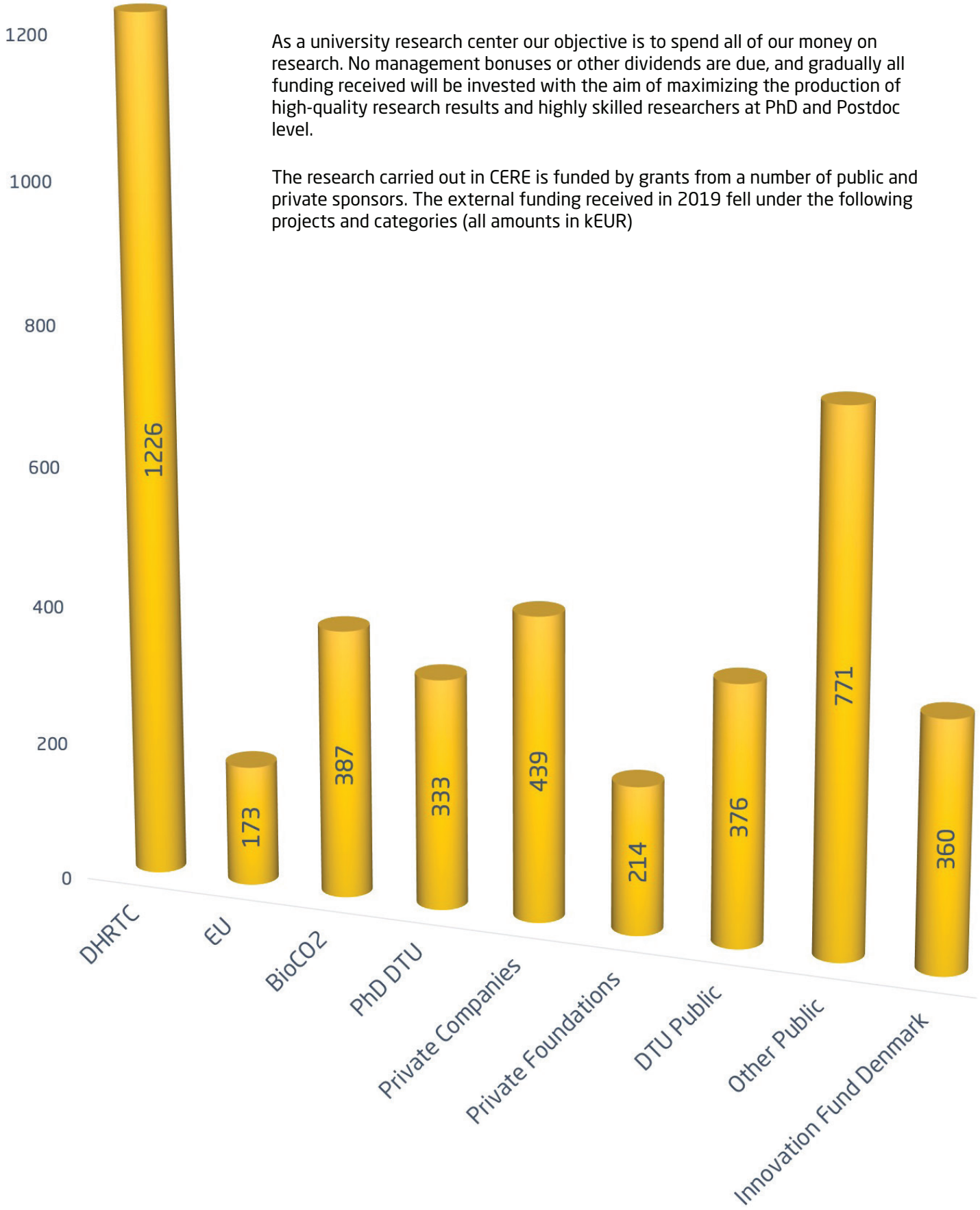
The microbial enrichment was found to drive a drastic reduction of complexity in the community structure, allowing for the selection of the microbial trophic groups of interest and conditioning the catabolic routes used by the microbial community. The production of ethanol and methane were used as target products for evaluating the potential control. For ethanol, a maximum yield of 59.15 ±0.18 % of the theoretical maximum was achieved. In the case of the production of methane, while the mesophilic enriched microbial community presented an intricate metabolic network and low specific CH4 productivity (1.83 ±0.27 mmol CH4/g VSS/h), the thermophilic enriched microbial community resulted in a much simpler community structure and a much higher specific CH4 productivity (33.48 ±0.90 nmol CH4/g VSS/h). Overall, microbial enrichments were found to be very effective for driving changes in the metabolic activity of microbial communities based on mutual exclusion interactions.

Analyzing the interspecies metabolic network based on the thermodynamic feasibility of prevailing net reactions during the fermentation of syngas alleviated partially the limitations of microbial enrichments, as it allowed for a more rational design of operational strategies targeting specific metabolic activities. Using this approach, increasing the initial concentration of acetate in the fermentation broth resulted in an increase of the maximum ethanol yield obtained in pH-based enrichments of acetogenic microbial communities by 22.5 % (reaching 72.44 ±2.11 % of the theoretical maximum).he mesophilic and thermophilic syngas fermentation process was modelled by integrating kinetic and thermodynamic considerations for simulating the performance of the microbial communities used. These models allowed for an accurate description of the methane productivity of these complex microbial systems via the simulation of the main microbial interactions. Several operational strategies for controlling the metabolism of the microbial communities were also identified through model simulations. In conclusion, the study suggests that combination of a range of tools is necessary for achieving improved control over the metabolic activity of microbial communities and thermodynamics hold a vital role in this respect.



Microbial enrichment and bioaugmentation techniques

Research Funding 2019



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

The research carried out in CERE is funded by grants from a number of public and private sponsors. The external funding received in 2019 fell under the following projects and categories (all amounts in kEUR)

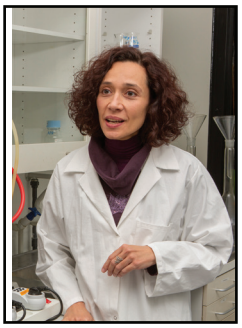
STAFF
Faculty

Arne Døssing Andreasen
DTU Space

Allan Peter Engsig-Karup
DTU Compute

Ida Lykke Fabricius
DTU Civil Engineering

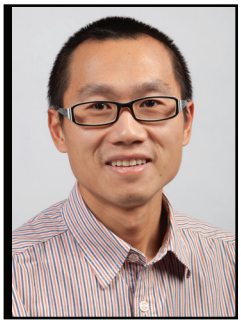
Philip Fosbøl
DTU Chemical Engineering



Hariklia Gavala
DTU Chemical Engineering

John Bagterp
DTU Compute

Georgios Kontogeorgis
DTU Chemical Engineering



Xiaodong Liang
DTU Chemical Engineering

Thomas G. Petersen
DTU Civil Engineering

Alexander Shapiro
DTU Chemical Engineering

Erling H. Stenby
DTU Chemistry

Kaj Thomsen
DTU Chemical Engineering

Nicolas von Solms
DTU Chemical Engineering

Wei Yan
DTU Chemistry

Michael L. Michelsen
(Emeritus)
DTU Chemical Engineering

Administrative Staff

Anne Louise Biede
DTU Chemical Engineering

Christian Ove Carlsson
DTU Chemical Engineering

Patricia Wagner
DTU Chemical Engineering

Klaus Mosegaard
(Associated Faculty)
Niels Bohr Institue

Technical Staff

Povl Valdemar Andersen, DTU Chemical Engineering
Thoung Dang, DTU Chemical Engineering
Morten Leth Hjuler, DTU Civil Engineering
Sinh Hy Nguyen, DTU Environment
Zacarias Tecle, DTU Chemical Engineering
John Troelsen, DTU Civil Engineering
Ditte Jul Valentin, DTU Civil Engineering
Maria del Pilar C. Vidal, Civil Engineering
Duc Thuong Vu, DTU Chemical Engineering

Scientific Staff

Susana Almeida, DTU Chemical Engineering
Alay Aria, DTU Chemical Engineering
Muhammad Waseem Arshad, DTU Chemical Engineering
Michael Bache, DTU Chemical Engineering
Nikolaj Blom, DTU Chemical Engineering
Yuan Chen, DTU Chemical Engineering
Christina Etler, DTU Chemical Engineering
Carolina Figueroa, DTU Chemical Engineering
Carsten F. Frøstrup, DTU Chemical Engineering
Andrew Holster, DTU Chemical Engineering
Jirigalatu Jirigalatu, DTU Space
Ida Arendt Kirknel, DTU Chemical Engineering
Nomiki Kottaki, DTU Chemical Engineering
Vamsi Krishna, DTU Space
Johan Kronholm, DTU Chemical Engineering
Xiaoyan Liu, DTU Chemistry
Isaac Løge, DTU Chemical Engineering
Leonardo Meireles, DTU Civil Engineering
Teresa Regueira Muniz, DTU Chemistry
Troels Nandrup-Bus, DTU Chemical Engineering
Randi Neerup, DTU Chemical Engineering
Zahra Nickmand, DTU Chemical Engineering
Martin Due Olsen, DTU Chemical Engineering
Tobias Orlander, DTU Civil Engineering
Ivanka Orozova-Bekkevold, DTU Civil Engineering
Duncan Paterson, DTU Chemistry
Diego Sandoval, DTU Chemistry
Eduardo Lima Simoes da Silva, DTU Space
Humbul Suleman, DTU Chemical Enginering
Christos Tsanos, DTU Chemistry
Athanasios Antonios Varsos, DTU Chemical Engineering
Guoliang Wang, DTU Chemical Engineering
Tian Wang, DTU Chemical Engineering
Rebecka M.L. Werchmeister, DTU Chemistry
Yi Yang, DTU Chemistry

PhD Students

Wael Almasri Al-Masri, DTU Chemical Engineering
Antonio Alemany, DTU Chemical Engineering
Justin Brand, DTU Chemical Engineering
Yingjun Cai, DTU Chemical Engineering
Edgar Camacho, DTU Chemical Engineering
Lasse Hjuler Christiansen, DTU Compute
Lucas F.F. Corrêa, DTU Chemical Engineering
Anna Burniol Figols, DTU Chemical Engineering
Wentao Gong, DTU Chemical Engineering
Casper Schytte Hemmingsen, DTU Mechanics
Steen Hørsholt, DTU Compute
Sarouyeh Khoshkolgh, Niels Bohr Institute
Mick Emil Kolster, DTU Space
Francois Kruger, DTU Chemical Engineering
Yigun Liu, DTU Chemistry
Petter Lomsøy, DTU Chemical Engineering
Fernando Medeiros, DTU Chemistry
Xianglei Meng, DTU Chemical Engineering
Henrik Lund Nielsen, DTU Chemical Engineering
Laura Paci, DTU Civil Engineering
Jyoti Pandey, DTU Chemical Engineering
Lisa Pasquinelli, DTU Civil Engineering
Amirali Rezazadeh, DTU Chemical Engineering
Anders Schlaikjer, DTU Chemical Engineering
Meng Shi, DTU Chemical Engineering
Einar Madsen Storebø, DTU Civil Engineering
Li Sun, DTU Chemical Engineering
Jihuan Tong, DTU Chemical Engineering
Mauro Torli, DTU Chemical Engineering
Evangelis Tsochantaris, DTU Chemical Engineering
Sebastian N.B. Villadsen, DTU Mechanical Engineering
Mark David Wigh, DTU Space
Yibo Yang, DTU Chemistry

External PhD Students

Yiqiu Chen, DTU Chemical Engineering
Markus Enekvist, DTU Chemical Engineering
Nipun Garg, DTU Chemical Engineering
Jiasheng Hao, DHRTC
Spardha Virendra Jhamb, DTU Chemical Engineering
Xinyan Liu, DTU Chemical Engineering
Yanrong Liu, DTU Chemistry
Olivia Ana Perederic, DTU Chemical Engineering
Mirhossein Taheriogtaghsara, DHRTC

External / Associated Staff

Irene Rocchi, DTU Civil Engineering
Jens Honore Walther, DTU Mechanics

Guests

Henrik Bohr, DTU Chemical Engineering
Jing Cai, DTU Chemical Engineering
Yang Lei, DTU Chemistry
Chenyang Zhu, DTU Chemical Engineering

Student Workers

Jakub Srna, DTU Chemical Engineering

Publications

Published in 2019

CERE 1709
"A massively scalable distributed multigrid framework for nonlinear marine hydrodynamics"
S.L. Glimberg, A.P. Ensig-Karup, and Luke N. Olson
(International Journal of High Performance Computing Applications, 33, (2019) 855-868)

CERE 1841
"Calculation of multiphase chemical equilibrium in electrolyte with non-stoichiometric methods"
Christos Tsanas, Erling H. Stenby, and Wei Yan
(Fluid Phase Equilibria, 482 (2019) 81-98)

CERE 1862
"Mechanisms of smart waterflooding in carbonate oil reservoirs – a review"
Jiasheng Hao, Samira Mohammadkhani, Hamidreza Shahverdi, Mohsen Nasr Esfahny, and Alexander Shapiro
(Journal of Petroleum Science and Engineering, 179 (2019) 276-291)

CERE 1870
"A Multiscale Direct Solver for the Approximation of Flows in High Contrast Porous Media"
Hani Akbari, Allan Ensig-Karup, Victor Ginting, and Felipe Pereira
(Journal of Computational and Applied Mathematics, 359 (2019) 88-101)

CERE 1901
"Accounting for cross association in non-self-associating species using a physically consistent SAFT-VR Mie approach"
Jamie T. Cripwell, Francois J. Kruger, and Andries J. Burger
(Fluid Phase Equilibria, 482 (2019) 1-13)

CERE 1902
"Dynamic Optimization of Thermodynamically Rigorous Models of Multiphase Flow in Porous Subsurface Oil Reservoirs"
Tobias K.S. Ritschel, and John Bagterp Jørgensen
(Journal of Process Control, 78 (2019) 45-56)

CERE 1903
"Enrichment of mesophilic and thermophilic mixed microbial consortia for syngas biomethanation: the role of kinetic and thermodynamic competition"
Antonio Grimalt-Alemany, Mateusz Łężyk, David M. Kennes-Veiga, Ioannis V. Skiadas and Hariklia N. Gavala
(Waste and Biomass Valorization, doi.org/10.1007/s12649-019-00595-z)

CERE 1904
"Modeling Tetra-n-butyl Ammonium Halides Aqueous Solutions with the Electrolyte CPA Equation of State"
Li Sun, Xiaodong Liang, Nicolas von Solms, Georgios M. Kontogeorgis
(Fluid Phase Equilibria, 486 (2019) 37-47)

CERE 1905A
"PρT Measurement and Modeling of n-decane+m-xylene Mixtures from 293.15 K to 363.15 K at Pressures up to 60 MPa"
Kai Kang, Xiaodong Liang, Georgios M. Kontogeorgis, and Xiaopo Wang
(The Journal of Chemical Thermodynamics, 135 (2019) 107-115)

CERE 1906
"Gas adsorption and Interfacial Tension with Classical Density Functional Theory"
Edgar L. Camacho Vergara, Georgios M. Kontogeorgis, and Xiaodong Liang
(Industrial Chemical Research, 58 (2019) 5650-5664)

CERE 1907
"Modelling of Wave-structure Interaction for Cylindrical Structures using a Spectral Element Multigrid Method"
Wojciech Laskowski, Harry B. Bingham, and Allan P. Ensig-Karup
(Presented at the 34th IWWWFB, Australia, 2019)

CERE 1910
"Pilot Scale Absorption Experiments with Carbonic Anhydrase-enhanced MDEA-Benchmarking with 30 wt% MEA"
Arne Gladis, Niels F. Lomholdt, Philip L. Fosbøl, John M. Woodley, and Nicolas von Solms
(International Journal of Greenhouse Gas Control, 82 (2019) 69-85)

CERE 1911
"Efficient transformation of CO_2 to cyclic carbonates using bifunctional protic ionic liquids under mild conditions"
Xianglei Meng, Zhaoyang Ju, Suojiang Zhang, Xiaodong Liang, Nicolas von Solms, Xiaochun Zhang, and Xiangping Zhang
(Green Chem. 21 (2019) 3456-3463)

CERE 1912
"Challenges in the development of a database of thermophysical properties of nanofluids"
M.E. Mondejar, M. Regidor, G. Kontogeorgis, and F. Haglind
(Presented at 1st International Conference on Nanofluids (ICNf2019), 2nd European Symposium on Nanofluids (ENSNf2019), 26-28 June, 2019, Castelló, Spain)

CERE 1914
"Investigation of the growth kinetics of tetra-n-butylammonium bromide hydrate formation in small spaces"
Meng Shi, Xuemei Lang, Yanhong Wang, Nicolas von Solms, and Shuanshi Fan
(American Chemical Society, 33 (2019) 3473-3482)

CERE 1918
"Bicarbonate flooding of homogeneous and heterogeneous cores from a carbonaceous petroleum reservoir"
Samira Mohammadkhani, Hamidreza Shahverdi, Sidsel Marie Nielsen, Mohsen Nasr Esfahany, and Alexander Shapiro
(Journal of Petroleum Science and Engineering, 178 (2019) 251-261)

CERE 1919
"Taking another look at the van der Waals equation of state – Almost 150 years later"
Georgios M. Kontogeorgis, Romain Privat, and Jean-Noël Jaubert
(Journal of Chemical and Engineering Data, 64 (2019) 4619-4637)

CERE 1920
"Solid solubility in the aqueous 2-amino-2-methyl-propanol (AMP) plus piperazine (PZ) system"
Randi Neerup, Kenny Ståhl, and Philip L. Fosbøl
(Journal of Chemical and Engineering Data, 64 (2019) 2423-2428)

CERE 1921
"High-pressure densities of n-decane+o-xylene mixtures: Measurement and modelling"
Kai Kang, Shanshan Zhu, Xiaodong Liang, Georgios M. Kontogeorgis, and Xiaopo Wang
(Fluid Phase Equilibria, 498 (2019) 1-8)

CERE 1922
"Insights into the solvation and dynamic behaviors of a lithium salt in organic- and ionic liquid-based electrolytes"
Jiahuan Tong, Xingqing Xiao, Xiaodong Liang, Nicolas von Solms, Feng Huo, Hongyan He, and Suojiang Zhang
(Physical Chemistry Chemical Physics, 21 (2019) 19216-19225)

CERE 1923
"Thermodynamic and kinetic properties of NH3-K2CO3-CO2-H2O system for carbon capture applications"
Stefano Lillia, Davide Bonalumi, Philip L. Fosbøl, Kaj Thomsen, Indira Jayaweera, and Gianluca Valenti
(International Journal of Greenhouse Gas Control, 85 (2019) 121-131)

CERE 1924
"Experimental studies on hydrogen hydrate with tetrahydrofuran by differential scanning calorimeter and in-situ Raman"
Jing Cai, Yuan-Qing Tao, Nicolas von Solms, Chun-Gang Xu, Zhao-Yang Chen, Xiao-Sen Li
(Applied Energy, 243 (2019) 1-9)

CERE 1925
"Modelling the critical and phase equilibrium properties of pure fluids and mixtures with the crossover Cubic-Plus-Association Equation of State"
Andre P.C.M. Vinhal, Wei Yan, and Georgios M. Kontogeorgis (Journal of Chemical and Engineering Data, (2019 DOI:10.1021/acs.jced.9b00492)

CERE 1926
"High-pressure experimental vapour-liquid-liquid equilibrium measurements and modelling for natural gas processing: Equipment validation, and the system CH4+nC6H14+H2O"
Francois Kruger, Athanasios A. Varsos, Georgios M. Kontogeorgis, and Nicolas von Solms
(Fluid Phase Equilibria, 501 (2019) 112276)

CERE 1927
"Hydrate stability and methane recovery from gas hydrate through CH4-CO2 replacement in different mass transfer scenarios"
Jyoti Shanker Pandey and Nicolas von Solms
(Energies, 12 (2019) 2309 -)

CERE 1928
"Experimental study of the phase behavior of hydrocarbon fluids in porous media at atmospheric and elevated pressures"
Teresa Regueira, Diego R. Sandoval, Erling H. Stenby, and Wei Yan
(Presented at Unconventional Resources Technology Conference (URTeC), Denver, Colorado, USA, 22-24 July 2019, DOI: 10.15530/urtec-2019-534)

CERE 1929
"Modeling of gas solubility using the electrolyte Cubic-Plus-Association Equation of State"
Li Sun, Georgios M. Kontogeorgis, Nicolas von Solms, and Xiaodong Liang
(Industrial and Engineering Chemistry Research, 58 (2019) 17555-17567)

CERE 1930
"Inhibition of methane hydrate nucleation and growth by an antifreeze protein"
Liang Mu, Hans Ramløv, T. Max M. Søgaard, Thomas Jørgensen, Willem A. de Jongh, and Nicolas von Solms
(Journal of Petroleum Science and Engineering, 183 (2019) 106388)

CERE 1932
"Insights into kinetics of methane hydrate formation in the presence of surfactants"
Jyoti Shanker Pandey, Yousef Jouljamal Daas, and Nicolas von Solms
(Processes, 7 (2019) 598; doi:10.3390/pr7090598)

CERE 1933
"Effect of compaction on oil recovery under low salinity flooding in homogeneous and heterogeneous chalk"
Jiasheng Hao, and Alexander Shapiro
(SPE-195831-MS, 2019)

CERE 1935
"Phase Equilibrium in shale including porous media effects"
Diego Rolando Sandoval Lemus, Wei Yan, and Erling H. Stenby
(Presented at Abu Dhabi International Petroleum Exhibition & Conference 2019, 11-14 November, 2019, United Arab Emirates)

CERE 1936
"Results of the fourth Technology Centre Mongstad campaign: LVC testing"
Philip Loldrup Fosbøl, Randi Neerup, Susana Almeida, Amirali Rezazadeh, Jozsef Gaspar, Anette Beate Nesse Knarvik, and Nina Enaasen Flø
(International Journal of Greenhouse Gas Control, 89 (2019) 52-64)

CERE 1937
"Process variables data from the lean vapour compressor campaign at Technology Centre Mongstad"
Philip Loldrup Fosbøl, Randi Neerup, Susana Almeida, Amirali Rezazadeh, Jozsef Gaspar, Anette Knarvik, and Nina Flø
(Data in Brief, 26 (2019) 104483-)

CERE 1943
"Development of nanoparticles as injection media in enhanced oil recovery"
Muhammad Waseem Arshad, Karen Louise Feilberg, Alexander Shapiro, and Kaj Thomsen
(SPE-198548-MS, 2019)

CERE 1944
"Methane hydrate formation behavior in the presence of selected amino acids"
Jyoti Shanker Pandey, Yousef Jouljamal Daas, and Nicolas von Solms
(Presented at the 8th International Conference on Chemical Science and Engineering (ICCSE 2019), Taipei, Taiwan, 18-20 November, 2019)

Submitted in 2019

CERE 1905B
"Support information to" "PρT Measurement and Modeling of n-decane+m-xylene Mixtures from 293.15 K to 363.15 K at Pressures up to 60 MPa"
Kai Kang, Xiaodong Liang, Georgios M. Kontogeorgis, and Xiaopo Wang

CERE 1908
"Application of response surface methodology for the optimization of aqueous ammonia soaking of wheat straw at ambient temperature for enhancing the methane yield"
A. Lymperatou, H.N. Gavala, and I.V. Skiadas

CERE 1913
"Equations of State in Three Centuries. Are we closer to arriving to a single model for all applications?"
Georgios M. Kontogeorgis, Xiaodong Liang, Alay Arya, and Ioannis Tsivintzelis

CERE 1917
"Multi-criteria optimization of process and refrigerant mixture for a small- scale natural gas liquefaction: enhancing energy efficiency, environmental benignness, and safety"
Saeed Eini, Georgios M. Kontogeorgis, Davood Rashtchian, and Mahdi Sharifzadeh

CERE 1934
"Density, compressibility and phase equilibrium of high pressure-high temperature reservoir fluids up to 473 K and 140 MPa"
Teresa Regueira, Maria-Lito Glykioti, Nomiki Kottaki, Erling H. Stenby, and Wei Yan

CERE 1940
"Supplementary Material – Cost optimization and flexibility analysis for the liquefaction of an associated natural gas stream"
Saeed Eini, Georgios M. Kontogeorgis, and Davood Rashtchian

CERE 1941
"Computer-aided design of paints and coatings"
Spardha Jhamb, Markus Enekvist, Xiaodong Liang, Xiangping Zhang, Kim Dam-Johansen, and Georgios Kontogeorgis

CERE 1942
"Modeling vapor-liquid-liquid-solid equilibrium for acetone-water-salt systems"
Kaj Thomsen, Martin Olsen, Lucas Corrêa

CERE 1945
"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

CERE 1946
"A new study of associating inhomogeneous fluids with classical density functional theory"
Edgar L. Camacho Vergara, Georgios M. Kontogeorgis and Xiaodong Liang

Conference contributions & Invited speakers, 2019

JANUARY

FEBRUARY

Minisymposium on Poroelasticity 2019, Bochum, Germany, 19 February 2019

T. Orlander, I. L. Fabricius, "Including temperature in the effective stress equation", Minisymposium on Poroelasticity 2019, Bochum, Germany, 19 February 2019 (Poster)

MARCH

Founders of Tomorrow, DTU Skylab, Denmark, 25 March 2019

Nikolaj Sorgenfrei Blom, "Being a disruptor in the quantum biology space", DTU Skylab, Denmark, 25 March 2019, (Invited speaker)

Sedimentary Gas Hydrate Workshop 2019, Linken Conference Center, Tromsø, Norway, 1-3 March 2019

Jyoti Shanker Pandey, "Kinetics of CH_4-CO_2 exchange in different mass transfer scenarios", Sedimentary Gas Hydrate Workshop 2019, Linken Conference Center, Tromsø, Norway, 1-3 March 2019, (Oral)

APRIL

East meets West Conference, Cracow, Poland, 9-12 April 2019

Sai Hema Bhavya Vinjarapu, Susana Almeida, Philip Loldrup Fosbøl, "Use of ultrasound for desorption of CO2 from MEA solution", East meets West Conference, Cracow, Poland, 9-12 April 2019, (Poster)

5th International Workshop on Rock Physics, Hong Kong, 23-26 April 2019

T. Orlander, K.A. Andreassen, I. L. Fabricius, "Stiffening by increased temperature of dry North Sea sandstones", 5th International Workshop on Rock Physics, Hong Kong, 23-26 April 2019 (Poster)

6th EAGE Shale Workshop, Bordeaux, France, 28 April-3 May 2019

I. Orozova-Bekkevold and T.G. Petersen, "Forward modelling of the evolution of shale properties in geological time", 6th EAGE Shale Workshop, Bordeaux, France, 28 April-3 May 2019, (Poster)

International Conference on Properties and Phase Equilibria for Product and Process Design 2019, (PPEPPD2019), Vancouver, Canada, 12-16 May 2019

Georgios Kontogeorgis, "Current status and challenges in electrolyte thermodynamics", International Conference on Properties and Phase Equilibria for Product and Process Design 2019, (PPEPPD2019), Vancouver, Canada, 12-16 May 2019, (Oral)

Edgar L. Camacho V., Georgios M. Kontogeorgis, Xiaodong Liang, "Advances in the Study of Inhomogeneous Fluids with Classical Density Functional Theory", International Conference on Properties and Phase Equilibria for Product and Process Design 2019, (PPEPPD2019), Vancouver, Canada, 12-16 May, (Poster)

Xiaodong Liang, Michael Locht Michelsen, Georgios M. Kontogeorgis, "The density gradient theory in surface tension calculations", International Conference on Properties and Phase Equilibria for Product and Process Design 2019, (PPEPPD2019), Vancouver, Canada, 12-16 May 2019, (Poster)

Xiaodong Liang, "PT flash calculations with cubic and association equations of state", International Conference on Properties and Phase Equilibria for Product and Process Design 2019, (PPEPPD2019), Vancouver, Canada, 12-16 May 2019, (Poster)

Xiaodong Liang, Georgios M. Kontogeorgis, "A MATLAB tool for teaching CPA and PC-SAFT", (Poster)

6th International Conference on Renewable Energy - Gas Technology, Malmo, Sweden, 20-21 May 2019

K. Asimakopoulos, A. Melas, H. N. Gavala, I. V. Skiadas, "Syngas Biomethanation by Mixed Microbial Consortia in Trickle Bed Reactors", 6th International Conference on Renewable Energy - Gas Technology, Malmo, Sweden, 20-21 May 2019, (Poster - book of abstracts of the 6th International Conference on Renewable Energy - Gas Technology)

DHRTC Young Researcher Day 2019, Technical University of Denmark (DTU), Kgs. Lyngby, Denmark, 24 May, 2019

Tian Wang, Simon Ivar Andersen, Alexander Shapiro, "Microfluidics study of the movement of oil droplets in thin capillaries", DHRTC Young Researcher Day 2019, Technical University of Denmark (DTU), Kgs. Lyngby, Denmark, 24 May, 2019 (Poster)

T. Regueira, D.R. Sandoval, E.H. Stenby, W. Yan, "Phase behaviour of n-alkanes in tight Lower Cretaceous formation", DHRTC Young Researcher Day 2019, Technical University of Denmark (DTU), Kgs. Lyngby, Denmark, 24 May 2019, (Poster)

JUNE

EAGE 81st Annual Conference and Exhibition, London, UK, 3-6 June 2019

Jiasheng Hao, Samira Mohammadkhani, Alexander Shapiro, "Smart Waterflooding of Homogeneous and Heterogeneous Cores in Carbonaceous Reservoirs", EAGE 81st Annual Conference and Exhibition, London, UK, 3-6 June 2019.

Summer School and Workshop in Calorimetry and Thermal Analysis 2019, 16-21 June, 2019

Jyoti Shanker Pandey, "Methane hydrate formation and dissociation behavior in the presence of selected amino acids", Summer School and Workshop in Calorimetry and Thermal Analysis 2019, 16-21 June, 2019, (Poster)

Trondheim CCS conference (TCCS-10), Trondheim, Norway, 17-19 June 2019

Sai Hema Bhavya Vinjarapu, Susana Almeida, Philip Loldrup Fosbøl, "Ultrasound assisted desorption of CO2 from MEA solution in the presence of VRAs", Trondheim CCS conference (TCCS-10), Trondheim, Norway, 17-19 June 2019, (Poster)

Ameya Joshi, Grégoire Dupont, Laurette Madelaine, Kaj Thomsen, Philip L. Fosbøl, "Measurement and Modeling of CO2 solubility in MEA solutions with additives", Trondheim CCS conference (TCCS-10), Trondheim, Norway, 17-19 June 2019, (Poster)

Sai Hema Bhavya Vinjarapu, Randi Neerup, Susana Raquel Melo de Almeida, Philip Loldrup Fosbøl, "Chemical kinetics of absorption of CO_2 by MEA in the presence of VRAs", Trondheim CCS conference (TCCS-10), Trondheim, Norway, 17-19 June 2019, (Poster)

Jens Kristian Jørsboe, Dennis Skov Kloth, Susana Almeida, Randi Neerup, Arne Gladis, Philip L. Fosbøl, "Impact of additives on CO2 capture in pilot scale for biogas upgrading",

Trondheim CCS conference (TCCS-10), Trondheim, Norway, 17-19 June 2019, (Poster)

Susana Almeida, Kaj Thomsen, Rasmus Find, Niels Z. R. Larsen, Jan F. Poulsen, Per G. Kristensen, Philip L. Fosbøl, "BioCO2, a project for improved low cost biogas upgrading and pure CO2 production", Trondheim CCS conference (TCCS-10), Trondheim, Norway, 17-19 June 2019, (Poster)

Dennis Skov Kloth, Randi Neerup, Susana Almeida, Philip Loldrup Fosbøl, "Solid-liquid equilibria of 30 wt% aqueous monoethanolamine (MEA) solution containing Vapour Reduction Additives (VRA)", Trondheim CCS conference (TCCS-10), Trondheim, Norway, 17-19 June 2019, (Poster)

Philip L. Fosbøl, Randi Neerup, Susana Almeida, Amirali Rezazadeh, Jozsef Gaspar, Anette Knarvik, Nina Flø, "Testing of the Lean Vapour Compressor (LVC) at Technology Centre Mongstad (TCM)", Trondheim CCS conference (TCCS-10), Trondheim, Norway, 17-19 June 2019, (Poster)

Randi Neerup, Sebastian Nis Bay Villadsen, Kaj Thomsen, and Philip Loldrup Fosbøl, "Thermodynamic Modelling of an Oxidative Biogas Cleaning System using the Extended UNIQUAC Model", Trondheim CCS conference (TCCS-10), Trondheim, Norway, 17-19 June 2019, (Poster)

JULY

NCSR "Demokritos" Summer school - scholarships and post-graduate studies, Demokritos, Greece, 10 July 2019

Georgios Kontogeorgis, "Job opportunities at the Technical University of Denmark related to a recent project from the European Research Council", NCSR "Demokritos" Summer school - scholarships and post-graduate studies, Demokritos, Greece, 10 July 2019 (Oral)

Unconventional Resources Technology Conference (URTeC), Denver, Colorado, USA, 22-24 July 2019

Teresa Regueira, Diego R. Sandoval, Erling H. Stenby, Wei Yan, "Experimental study of the phase behavior of hydrocarbon fluids in porous media at atmospheric and elevated pressures", Unconventional Resources Technology Conference (URTeC), Denver, Colorado, USA, 22-24 July 2019 (Oral); DOI 10.15530/urtec-2019-534

DAREDISRUPT Fireside chat for Mærsk Drilling, Copenhagen, Denmark, 2 July 2019

Nikolaj Sorgenfrei Blom, "Water as the new wind?" DAREDISRUPT Fireside chat for Mærsk Drilling, Copenhagen, Denmark, 2 July, 2019, (Invited speaker)

International Chemistry Congress (IUPAC, 2019), France 5-12 July 2019

Jyoti Shanker Pandey, "Insights into CO_2 capture by flue gas hydrate formation using selected Amino acids and surfactants", International Chemistry Congress (IUPAC, 2019), France 5-12 July 2019, (Oral)

AUGUST

36th International Conference on Solution Chemistry (36 ICSC), Xining, China, 4-8 August 2019

Li Sun, "Modeling of gas solubility using the e-CPA equation of state", 36th International Conference on Solution Chemistry (36 ICSC), Xining, China, 4-8 August 2019, (Oral)

Kaj Thomsen, Martin Due Olsen, "Modeling phase equilibria of acetone – water – salt mixtures", 36th International Conference on Solution Chemistry (36 ICSC), Xining, China, (Oral)

Society of Core Analysts Annual Symposium 2019 Pau, France 25-30 August 2019

Jyoti Shanker Pandey, "Methane production through combined depressurization + hydrate swapping method in the Sandy porous medium under permafrost temperature conditions, Society of Core Analysts Annual Symposium 2019 Pau, France 25th August -30th August 2019 (Short oral and poster)

SEPTEMBER

12th European Congress of Chemical Engineering (ECCE12) joint with 5th European Congress of Applied Biotechnology (ECAB5), 15-19 September 2019, Florence, Italy

Olivia Perederic, Bent Sarup, John M. Woodley, G.M. Kontogeorgis, "Systematic computer aided methods and tools for lipid process technology", 12th European Congress of Chemical Engineering (ECCE12) joint with 5th European Congress of Applied Biotechnology (ECAB5), 15-19 September 2019, Florence, Italy, (oral Presentation)

Xinyan Liu, Xiangping Zhang, Zhang Suojiang, Xiaodong Liang, Rafiqul Gani, Georgios M. Kontogeorgis, "Ionic liquid design and process simulation for shale gas separation", 12th European Congress of Chemical Engineering (ECCE12) joint with 5th European Congress of Applied Biotechnology (ECAB5), 15-19 September 2019, Florence, Italy, (poster)

Yiqun Liu, Teresa Regueira, Erling Halfdan Stenby, Wei Yan, "Phase equilibrium and density of highly asymmetric gas-oil mixtures at high temperatures and high pressures", 12th European Congress of Chemical Engineering (ECCE12) joint with 5th European Congress of Applied Biotechnology (ECAB5), 15-19 September 2019, Florence, Italy, (poster)

International Energy Agency Enhanced Oil Recovery Conference (4th EOR TCP), Cartagena, Colombia, 16-20 September 2019

Samira Mohammadkhani, Jiasheng Hao, Alexander Shapiro, "Impact of Heterogeneity on Smart Waterflooding in Carbonaceous Rocks", International Energy Agency Enhanced Oil Recovery Conference (4th EOR TCP), Cartagena, Colombia, 16-20 September 2019

10th European Symposium on Biopolymers, Straubing, Germany, 25-27 September 2019

A. Burniol-Figols, I. V. Skiadas, A. E. Daugaard, H. N. Gavala, "Polyhydroxyalkanoates (PHA) purification through dilute aqueous ammonia digestion at elevated temperatures", 10th European Symposium on Biopolymers, Straubing, Germany, 25-27 September 2019, (Oral – book of abstracts, 10th European Symposium on Biopolymers)

SPE Annual Technical Conference and Exhibition, Calgary Alberta, Canada, 30 September-2 October 2019

Jiasheng Hao and Alexander Shapiro, "Effect of Compaction on Oil Recovery under Low Salinity Flooding in Homogeneous and Heterogeneous Chalk", SPE Annual Technical Conference and Exhibition, Calgary Alberta, Canada, 30 September-2 October 2019, (Oral and SPE 195831)

OCTOBER

DAREDISRUPT Fireside chat for HAFSLUND (Norway), Copenhagen, Denmark, 10 October 2019

Nikolaj Sorgenfrei Blom, "Water as the new wind?", DAREDISTUPT Fireside chat for HAFSLUND (Norway), Copenhagen, Denmark, 10 October 2019, (Invited speaker)

Tsinghua University, Tsinghua, China, 14 October 2019

Georgios Kontogeorgis, "Equations of state in three centuries – What have we learnt? What more needs to be done?", Tsinghua University, Tsinghua, China, 14 October 2019, (Invited lecture)

Institute of Process Engineering, (IPE), Chinese Academy of Sciences, Beijing, China, 16 October, 2019

Georgios Kontogeorgis, "Advanced Thermodynamic Models. But how much have we advanced Science and Engineering?", Institute of Process Engineering, (IPE), Chinese Academy of Sciences, China, 16 October 2019 (Invited lecture)

1st International Green and Sustainable Chemistry Conference, Beijing, China, 17-19 October 2019

Xiaodong Liang, Georgios M. Kontogeorgis, "Equation of state models for green chemical engineering", 1st International Green and Sustainable Chemistry Conference, Beijing, China, 17-19 October 2019, (Oral)

14th Annual Conference on the Physics, Chemistry and Biology of Water, Bad Soden, Germany 24-27 October 2019

Nikolaj Sorgenfrei Blom, "Water as the new wind?", 14th Annual Conference on the Physics, Chemistry and Biology of Water, Bad Soden, Germany 24-27 October 2019

NOVEMBER

DAREDISRUPT Fireside chat for Maritime Disruptor Academy, Copenhagen, Denmark 2019

Nikolaj Sorgenfrei Blom, "The future of energy is water", DAREDISRUPT Fireside chat for Maritime Disruptor Academy, Copenhagen, Denmark 2019, (Invited speaker)

DHRTC Technology Conference 2019, Kolding, Denmark, 5-6 November 2019

Hadise Baghooee, François Montel, Charlotte Lassen, Wei Yan, Alexander Shapiro, "Thermal Segregation in Petroleum Reservoirs", DHRTC Technology Conference 2019, Kolding, Denmark, 5-6 November 2019 (poster)

I. Orozova-Bekkevold, T. G. Petersen, "The role of permeability in compaction and overpressure build-up during deposition", DHRTC Technology Conference 2019, Kolding, Denmark, 5-6 November 2019, (Poster)

Tian Wang, Simon Ivar Andersen, Alexander Shapiro, "Microfluidic study of oil droplets in microchannels", DHRTC Technology Conference 2019, Kolding, Denmark, 5-6 November 2019, (Poster)

T. Regueira, R.M.L. Werchmeister, E. H. Stenby, W. Yan, "PVT study of a Lower Cretaceous live fluid for gas injection", DHRTC Technology Conference 2019, Kolding, Denmark, 5-6 November 2019, (Poster)

T. Regueira, D.R. Sandoval, E.H. Stenby, W. Yan, "Phase behaviour of n-alkanes in tight Lower Cretaceous formation", DHRTC Technology Conference 2019, Kolding, Denmark, 5-6 November 2019, (Poster)

Zahra Nickmand and Nicolas von Solms, "Extended Reach Intervention by Polymer as Friction and Viscosity Reducer: An experimental study", DHRTC Technology Conference 2019, Kolding, Denmark, November 5-6, 2019, (Poster)

DHRTC Technology Conference 2019, Copenhagen, Denmark, 10-11 November 2019

H.F. Christensen, A. Shamsolhodaei, T. Orlander, "4D Seismics – input for optimized interpretation", DHRTC Technology Conference 2019, Copenhagen, Denmark, 10-11 November 2019 (Poster)

H.F. Christensen, A. Shamsolhodaei, T. Orlander, "Plug cleaning, classification, database and plug archive", DHRTC Technology Conference 2019, Copenhagen, Denmark, 10-11 November 2019 (Poster)

H.F. Christensen, A. Shamsolhodaei, T. Orlander, "Compaction and geomechanics testing", DHRTC Technology Conference 2019, Copenhagen, Denmark, 10-11 November 2019 (Oral)

8th International Conference on Chemical Science and Engineering (ICCSE 2019), National Taipei University of Technology, Taiwan, 18-20 November, 2019

Jyoti Shanker Pandey, "Methane hydrate formation behaviour in the presence of selected amino acids", 8th International Conference on Chemical Science and Engineering (ICCSE 2019), National Taipei University of Technology, Taiwan, 18-20 November, 2019, (oral and conference paper)

DECEMBER

2nd European Aquaphotomics Conference, Budapest, Hungary 2-3 December 2019

Nikolaj Sorgenfrei Blom, "DireWaves – Disarming resistant microbes with resonant waves", 2nd European Aquaphotomics Conference, Budapest, Hungary 2-3 December 2019, (Invited speaker)

3rd International Conference on Functional Materials and Chemical Engineering 2019 (ICFMCE 2019), Bangkok, Thailand, 15-17 December 2019

Olivia A. Perederic, Franjo Cecelja, John M. Woodley, Georgios M. Kontogeorgis, Antonis Kokossis, "Streams Property Characterisation in Waste Biorefineries Using an Ontology Approach", 3rd International Conference on Functional Materials and Chemical Engineering 2019 (ICFMCE 2019), Bangkok, Thailand, 15-17 December 2019, (Poster)

Technical University of Athens, Athens, Greece, 19 December 2019

Georgios Kontogeorgis, "Thermodynamics for a sustainable chemical engineering in a changing world", Technical University of Athens, Athens, Greece, 19 December 2019 (Invited lecture)