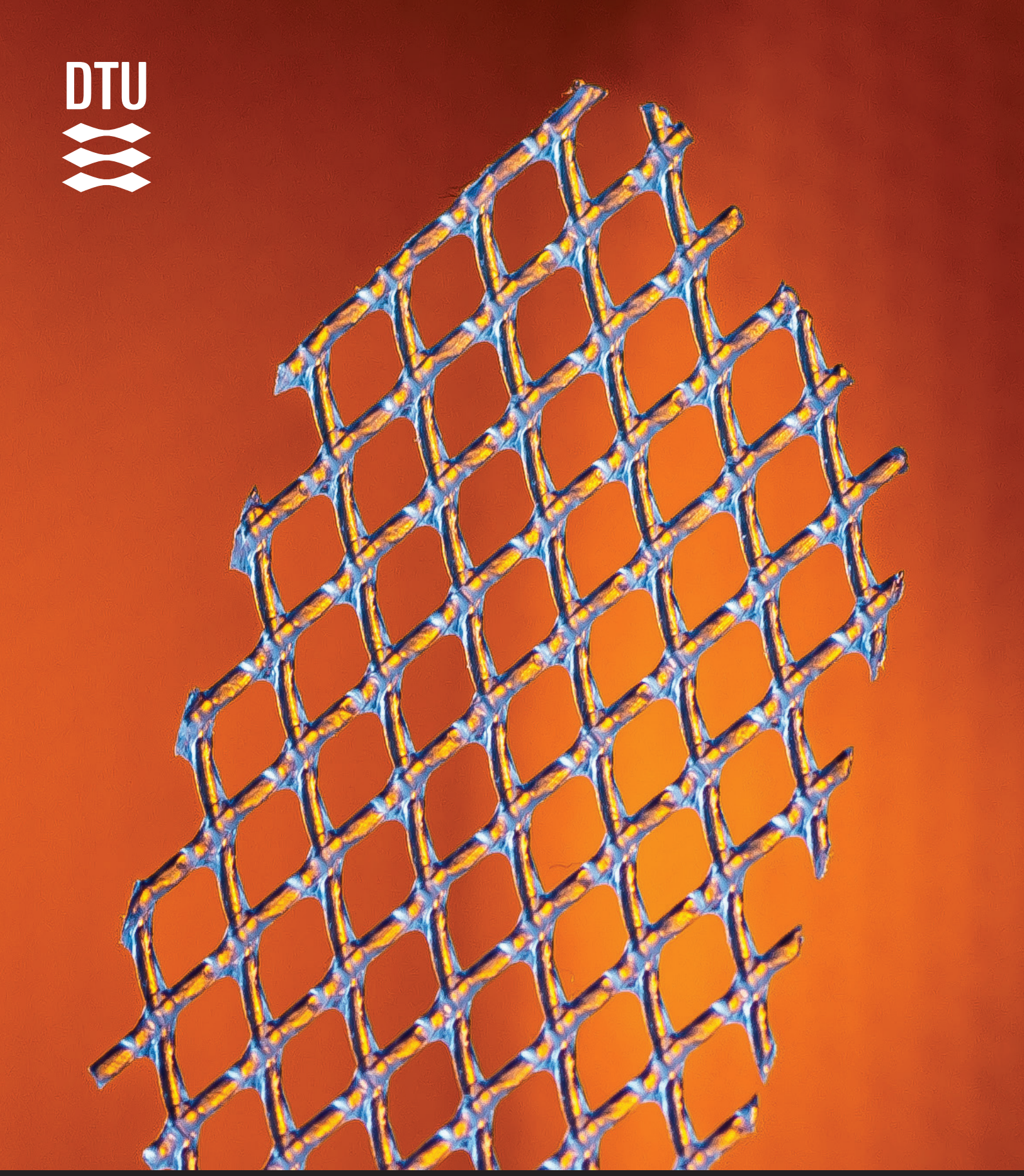
DTU



CERE Annual Report 2021

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Cover:
"The picture shows an insertion lattice to electrochemical cells, creating turbulence and enhancing mass transfer. We use electrochemistry in novel technologies to capture CO_2, which can significantly reduce the associated cost. CO_2 is captured in an alkaline solution, and with a potential gradient, the pH is lowered. As the pH decreases, CO_2 is released into a pure gas stream. A pure stream of CO_2 gas can be used or transported to a storage site."

CONTENT

INTRODUCTION

A return to dynamic normality

Research is a peculiar line of work. While so many other trades are heavily affected if not totally brought to a standstill when forced to close their physical premises, the wheels of academia somehow manage to keep turning. Looking at the production of CERE – be it scientific articles, flow of students, lectures, experimental activities, administrative work – one would never guess that we like the rest of the world have been subject to an epidemic or that access to our offices and laboratories was interrupted several times during the past two years.

So, in a general sense I can say that I have the pleasure of introducing a normal annual report. Still, normal doesn't mean business-as-usual.
A remarkable novelty of strategic significance in 2021 was seen in the field of carbon capture. Following an agreement in the Danish parliament by December 2021, Denmark is committed to create a market for carbon capture, utilization, and storage (CCUS) over the next few years. Leading up to the political accord was an intensive preparatory effort by a range of industrial and academic stakeholders with several CERE experts strongly involved.

Further, the carbon capture researchers at CERE will have a leading role in a major EU scheme aiming to test a novel capture technique at pilot plant scale in three different industries in Denmark, Greece, and Romania respectively. In other words, we are seeing a longstanding commitment from CERE over several decades paying off today.

A strong industrial Consortium

As we know, scientific progress rarely happens in a vacuum but rather is the result of the interaction between academic activities and practical implementation. On that account, I am confident we will see several breakthroughs in CCUS over the coming years. And already, we have seen one new member company, Dan-Unity, joining the CERE industry Consortium mainly due to potential CCUS collaborations. Dan-Unity is a shipping company specializing in transports related to carbon capture and storage.

The second new member company in 2021, AVEVA, is a global leader in industrial software, not least within process engineering and simulation software. Furthermore, we can welcome Schlumberger back as Consortium member after a short absence. As always, the strength and vitality of the Consortium is testament to the relevance of what we do.

Rounding off the remarks on CCUS, these activities are another confirmation of the rationale behind CERE as an interdisciplinary research center. Initially, the carbon capture activities at DTU were almost exclusively within chemical engineering but today they have a broader focus, not least with strong interdependencies with geology for the storage component, and with biotechnology for the utilization component.

Exciting interdisciplinary developments

Similarly, we see several exciting developments that originate from fields which border or interact with chemical engineering.

Researchers in CERE have contributed to a European project with huge potential impact: A novel technique recycles the polymer PET – the fourth largest polymer worldwide in terms of production quantity - back to its original monomers.

And, perhaps surprisingly, drones with magnetic surveying equipment can assist the ongoing offshore wind build-out. The drones identify unexploded bombs and mines from past wars, thereby reducing both a hazard and a large economic risk factor in offshore wind park construction.

In July 2021, the Government of Greenland decided to halt all hydrocarbon exploration. However, while oil and gas exploration in Greenland is off the table, seismic investigations conducted by the hydrocarbon industry over the most recent years may still be put to good use. The wealth of data from seismic investigations have opened the door to a better understanding of past climate changes. This again may help policy makers adapt to future climate events.

A relatively young research field for CERE is the behavior of water at the fundamental level. In a joint project with ferry operators Molslinjen, the CERE water research group has shown effects from electromagnetic modification of diesel fuel, and the group continues working on a range of both conventional and unconventional ideas.

Looking forward to seeing you in person

Thermodynamic modelling and simulation, a classic CERE stronghold, continue to be in excellent shape and at the core of our activity. CERE has the coordinating role in a major European project aiming to advance the understanding of electrolytes. The importance of electrolytes is growing in a variety of industrial and academic contexts.

Summing up, I hope to have demonstrated that CERE is as vital and relevant as ever. Still, I must admit that it has felt a bit strange to manage such a large proportion of both our internal and external relations remotely.

Video conferencing is here to stay, but we are planning to have more physical events – not least the CERE Discussion Meeting 2022. I believe that I can speak for all of us here at CERE, when I say that we look forward to seeing you all in person soon!

Professor Nicolas von Solms,
Chairman of CERE

Industry Consortium

The Consortium – our Strongest Asset

CERE is supported by public means from several sources, e.g. Innovation Fund Denmark, EU framework programs for science and innovation, and The Danish Research Councils. Furthermore, the center is supported by grants from several private companies. The strongest asset of CERE is the industrial Consortium. Currently 17 companies are members, the number changes due to the dynamics of the industry's mergers and acquisitions. The member companies closely follow the activities of our center. This ensures that CERE activities are relevant in relation to the topical problems and limitations in existing knowledge. This ongoing external control of quality and inspiration assist in maintaining CERE research at the highest international level.

We welcome **AVEVA**

AVEVA, a global leader in industrial software, has joined the CERE industry Consortium. The interests of AVEVA include process engineering and simulation software.

Through Performance Intelligence, AVEVA connects the power of information and Artificial Intelligence (AI) with human insight, to enable faster and more precise decision making, helping industries to boost operational delivery and sustainability.

AVEVA is headquartered in Cambridge, UK, with over 6,000 employees at 90 locations in more than 40 countries.

We welcome **Dan-Unity**

Shipping company Dan-Unity, specializing in transport related to carbon capture and storage, has joined the CERE industry Consortium.

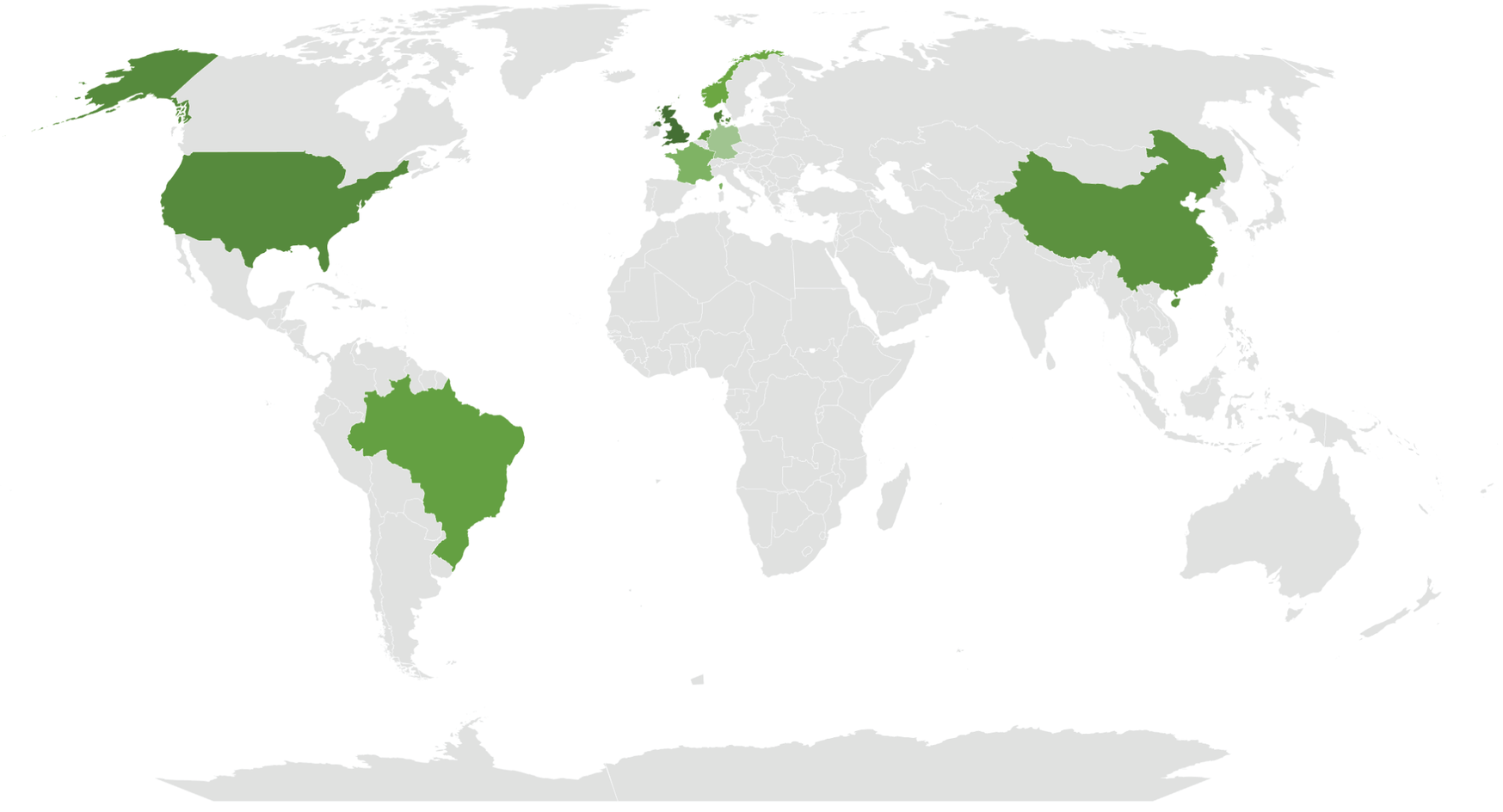
The company was established by Danish shipping companies Evergas and Ultragas, each market leaders within their respective segments of liquified gas transportation.

Evergas is one of the world's leading seaborne transporters of petrochemical gases and natural gas liquids. The company is headquartered in Copenhagen with offices in Singapore, Paris, and Shanghai.

Ultragas, also headquartered in Copenhagen, is a leading provider of marine transportation of liquefied petroleum and petrochemical gases. Ultragas is part of the Ultranav shipping group with offices in 15 countries.

With the establishment of Dan-Unity as their joint company, Evergas and Ultragas have created the world's first carbon capture and storage specific shipping entity.

CERE Consortium



Aveva
BP
Calsep
Chevron
China Petrochemical Technology Company Ltd
DSM
ESSS
Equinor
Dan-Unity
IFPEN
KBC/Infochem
Linde
Schlumberger
Shell
Total
Union Engineering - Pentair
Wintershall-DEA

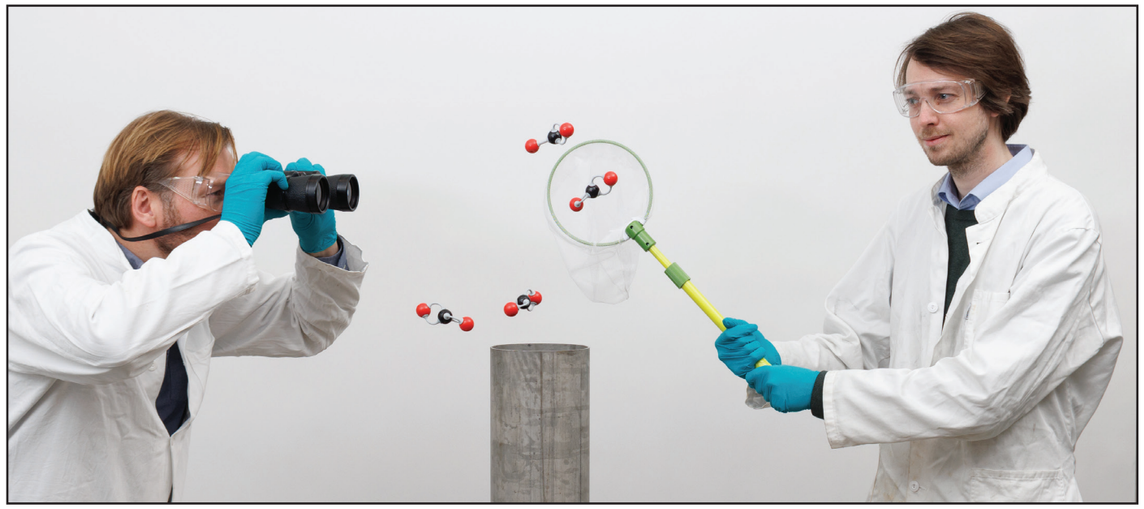
CARBON CAPTURE

Philip Loldrup Fosbøl

Sebastian Nis Bay Villadsen

Uffe Ditlev Bihlet

Major role in EU carbon capture project



Associate Professor Philip L. Fosbøl, heading the carbon capture group at CERE & Senior Project Manager Sebastian Nis Bay Villadsen, CERE

CERE will lead the construction of a mobile unit to demonstrate CO2 capture at industrial plants in Denmark, Greece, and Romania.

Three industrial plants in Denmark, Greece, and Romania become the sites for the first demonstrations of a new carbon capture technology based on alkali absorption coupled to a novel electrodialysis cell. The method could become an important alternative to the currently dominant absorption method which is amine-based solvents.

"The main advantage of the alkali absorption method is low energy consumption. Since energy costs weigh heavily in amine-based capture, this could be a gamechanger. The results obtained in the lab are at a disruptive level. The question now is whether we can obtain the same in the demonstration projects," says Senior Project Manager, Sebastian Nis Bay Villadsen, CERE.

The three upcoming demonstrations will take place at Aalborg Portland's cement production site, at the Yerakine Mine in Greece, and at OMV Petrom's Petrobrazi refinery

"The real revelation is that after capture, the CO_2 can easily be extracted from potassium hydroxide using electrodialysis."

Senior Project Manager Sebastian Nis Bay Villadsen, CERE.

in Romania respectively. The demonstrations are part of a larger EU-funded project named ConsenCUS on carbon capture use and storage (CCUS).

Carbon capture in caustic potash

The alkali absorption method is developed by Dutch technology center Wetsus, also a ConsenCUS partner.

"Wetsus has demonstrated the potential of the method in their labs. However, they need our expertise when it comes to upscaling. This is where we have decades of experience. Tests and experiments will run in parallel. Some in lab scale at the Wetsus facilities in The Netherlands, some at pilot scale here at DTU, and later at demonstration scale at the three industrial sites. We plan to have extensive knowledge sharing all the way. It is important that we coordinate the experiments so results can be compared," explains Associate Professor Philip L. Fosbøl, heading the carbon capture group at CERE.

In the Wetsus method, carbon capture takes place in potassium hydroxide solution, KOH. Still, the main advantage does not lie in the capture ability

itself, according to Sebastian Nis Bay Villadsen:

"Once you have captured CO_2 you need to extract the CO_2 from your solvent not only to either use or store the CO_2 but also, importantly, to regenerate your solvent. In amine-based capture this can only be achieved through a relatively large energy input. The real revelation by our Dutch colleagues is that the CO2 can easily be extracted from KOH using electrodialysis."

Remains strongly involved in amine capture

The group at CERE does not plan to abandon its activities in amine-based carbon capture. First and foremost, the group remains strongly committed through an existing mobile capture unit using amine-based solvents. The unit was currently in operation at waste incineration plant ARC (Amager Ressource Center and is now at a biogas plant in Hanshøj).

The amine-based unit is a cornerstone in the ambition of ARC to have full scale carbon capture implementation by 2025.

"It does not seem realistic for the alkali absorption to be ready for full scale implementation within such a short timeframe. After all, the amine-based techniques have been optimized through several decades of fine engineering," Sebastian Nis Bay Villadsen comments.

It would be premature to call a winning technology, notes Philip L. Fosbøl:

"If we succeed in lowering the energy costs, and thereby lower the costs of operating the capture units, a new dynamic will come into play. We will see a shift from focus on cost of operation to cost of building the capture units. This will involve questions like which materials are needed, what do they cost at the time, and will it be possible to use smaller amounts of materials through optimization."

A further issue will be the price of electric power versus the price of heat, adds Sebastian Nis Bay Villadsen:

"Amine-based units are normally able to use excess heat from nearby facilities, while the Wetsus method will need electric power. Historically, electric power has been more costly than heat, but this may change due to positive developments in wind power, solar power etc. These questions are all outside the scope of what we do in our group, but they may have a large impact when decisions are made on which technology to go for. In any case, we find it wise to engage in more than one capture technology."

Cement production, magnesite mining, oil refinery

In the project, a mobile unit will be built. The first demonstration is scheduled for Aalborg Portland's cement production site with likely inauguration by late 2023.

"Since a major part of the assembly work will take part here at DTU, it was natural to plan for the Danish site as the first place of demonstration," says Sebastian Nis Bay Villadsen. Once in operation, the Aalborg demonstration facility is planned to run for five months. The demonstration cycle will include a preliminary test and a parametric screening study.

Hereafter, the mobile unit will be moved to Greece and later to Romania, also operating five months at each of both these sites.

In Greece, the unit will be installed close to a rotary kiln at the Yerakini Mine in Chalkidiki. The mine is operated by Grecian Magnesite. Long-term test cycles will focus on solvent stability and accumulation of unwanted residues. The scope of the test cycles is to perform more than 1,000-hour tests.

In Romania, the unit will be installed at the OMV Petrom's Petrobrazi refinery. Long-term test cycles will focus on solvent stability and again, the aim is +1,000-hour tests.

Associate Professor Philip Loldrup Fosbøl visiting Aalborg Portland. The cement factory is one of the largest emitters of CO_2 in Denmark and part of the ConsenCUS project. Aalborg Portland are also active in developing the CCUS strategy in Denmark.

"Since the exhaust gases are quite different in cement production, in magnesite mining, and at a refinery, we will be able to test the technology under different, relevant conditions," notes Sebastian Nis Bay Villadsen.

Manages a third of the European budget

The overall budget of ConsenCUS is the equivalent of 100 million DKK. Hereof approximately half is for the technical demonstration projects, and the DTU team will manage the 34 million DKK.

It should be noted, that ConsenCUS is about more than technical demonstrations. The other half of the total budget is dedicated to other sides of CCUS, not least building industrial clusters and engage with local communities around CCUS. Further subprojects will include conversion of captured CO2 into formate and formic acid, and safe cyclic loading of CO2 into salt formations and aquifers for storage.

ConsenCUS is just the most recent example of the carbon capture group at CERE being part of a successful European consortium within CCUS. Over the latest two-three decades, the group has consistently taken part in all major EU programs in the field.

CERE in Danish capture partnership

Associate Professor Philip Loldrup Fosbøl, Project Manager Uffe Ditlev Bihlet and Senior Project Manager Sebastian Nis Bay Villadsen visiting the Greek ConsenCUS project partner Grecian Magnesite. The Greek mining site will host the carbon capture demonstration unit in 2024, as the final of 3 different demonstration sites.

A wide range of academic and industry partners have set out to create a Danish market for carbon capture utilization and storage (CCUS).

Partners from the universities, public sector research, industry, and the approved technological services institutes (GTS) have entered a wide-ranging innovation partnership on carbon capture, utilization, and storage (CCUS). Titled INNO-CCUS, the partnership is a consequence of a decision by the Danish parliament in December 2021 to devote 16 billion DKK for development of a market for CCUS. The first facilities are intended to become operational by 2025.

"For decades, we have extracted oil from the North Sea. This will become a thing of the past. Instead, we are to capture CO_2 and store it in the very same underground. Exactly this technology will be an important element in our 70 per cent target (reducing Danish CO_2 emissions by 70 per cent by 2030 relative to 1990). This is because carbon capture and storage may reduce emissions in certain sectors where reductions have proved very difficult to achieve. Examples are waste incineration and cement production. The potential is huge, and it is therefore important to kickstart the market now," said Dan Jørgensen, Danish Climate Minister when announcing the agreement.

A roadmap for Danish CCUS

According to the Danish government, CCUS has the potential to reduce the amount of CO_2 in the atmosphere by 4-9 million tons by 2030. However, even though some CCUS technologies are well known, interdisciplinary efforts, greater collaboration, more research, and large-scale testing are still needed. Therefore, a range of partners have joined forces, assisting the Danish government in designing a roadmap for the process ahead. Throughout 2021, several CERE faculty members and other staff have been active in the DTU contribution to the roadmap.

"CERE's strong track record within both capture and storage of CO_2 gives the center an important role in the new partnership," says Professor Erling H. Stenby who has coordinated DTU's role in the partnership.

The key purpose of the INNO-CCUS partnership is to implement the CCUS roadmap. The plan is to focus on short-term (2025), medium-term (2030), and long-term (2050) solutions that will contribute to Denmark achieving its climate goals while at the same time supporting the establishment of new green industries, export opportunities, growth, and research.

Secretariat at DTU

The partnership has identified several projects within five core areas: chemical carbon capture, biological carbon capture and storage, geological carbon storage, carbon utilization, social and system analysis.

The partnership and roadmap are supported by Innovation Fund Denmark which, based on the Danish Finance Act (Finanslov) 2021, has been tasked with investing a total of DKK 700 million in mission-driven green partnerships – including CCUS.

An interim eight-man board has been appointed for INNO-CCUS. Morten Stage, head of CCS at TotalEnergies, has been appointed chairman, while Professor Erling H. Stenby, CERE, has been appointed vice chairman. In addition, a secretariat for the partnership will be established at DTU.

The INNO-CCUS partners

Seven universities:

- Aalborg University
- Aarhus University
- Copenhagen Business School
- DTU
- University of Copenhagen,
- Roskilde University
- University of Southern Denmark.

Eight companies:

- Aalborg Portland
- ARC
- Gas Storage Denmark
- INEOS
- Novozymes
- Pentair
- TotalEnergies
- Ørsted.

One governmental research institution:

- Geological Survey of Denmark and Greenland (GEUS).

Four GTS institutes:

- The Danish Technological Institute (DTI),
- The Alexandra Institute
- DHI
- FORCE Technology.

One industrial cluster:

- Energy Cluster Denmark.

ELECTROLYTE SYSTEMS

Georgios M. Kontogeorgis

Saman Naseri Boroujeni

Martin Due Olsen

Advances in the understanding of electrolytes

Not least due to the expansion of bioprocessing, the importance of electrolytes is growing in a variety of industrial and academic contexts. This has called for development of new theory and improved understanding since thermodynamic models for electrolytes are more complex than the non-electrolyte ones, and much more difficult to use for practicing chemical engineers. There is lack of fundamental understanding for many aspects of electrolyte solutions. A European project is set up to meet the demand.

"We have a dual aim of improving the fundamental understanding of electrolyte thermodynamics and developing engineering models in the form of advanced equations of state suitable for electrolyte solutions," says Professor Georgios M. Kontogeorgis, CERE, Principal Investigator in the project "New Paradigm in Electrolyte Thermodynamics."

Water is the common denominator for many sub-projects, he adds:

"Water is the main component in many electrolyte solutions but currently even the most advanced models cannot describe water's special properties."

Accounting for ion pair effects

Sometimes a new paradigm may build on an old idea. In his project, PhD Researcher Saman Naseri Boroujeni, CERE, investigates a thought launched by the Danish scientist Niels Bjerrum more than 100 years ago. Namely, that since ions form anion/cation-pairs which exist in a solution for shorter or longer periods of time, electrolyte thermodynamics models should take ion-ion association into account. Bjerrum's idea did not catch momentum in his own time, but may well do so now, explains Saman Naseri Boroujeni:

"Not least will the conductivity of an electrolyte solution be strongly affected by the existence of ion pairs. The conductivity is often quite large due to the existence of ions, but if, say, 20 per cent of the ions are engaged in ion pairs these ions do not contribute to conductivity. Thus, if your model does not take ion-ion associations into account, it will overpredict conductivity accordingly."

Inaccurate prediction of con-

ductivity has further implications, he notes:

"Firstly, conductivity is highly important to several types of electrolyte solutions. One example is batteries, where a high level of conductivity is the key to achieving the rate of charging you aim for."

"Secondly, conductivity is one of the best tools we have at our disposal for many types of experiments. Studies of electrolyte solutions are often challenging. Seeing what happens as we apply current to the mixture will often give valuable information. But again, this only makes sense if what we see is the true order of the change in conductivity – with the effect of ion pairs accounted for."

Relevant to a range of industries

Including ion-ion associations in thermodynamic modelling is easier said than done, according to Saman Naseri Boroujeni:

"Experimental data for ion-ion associations are only available for a few systems. Therefore, we have had to include many different data sources – data from different types of spectroscopies etc. – and results from different thermodynamic models."

While the studies on ion-pairs and electrical conductivity are already published, Saman Naseri Boroujeni is determined to bring the concept closer to practical implementation:

"The aim is to have ion-ion association integrated into the e-CPA (electrolyte cubic plus association) model by the end of my PhD project. This innovation will be relevant for a range of industries within process engineering, chemical manufacturing, energy conversion, and others."

"Water is the main component in many electrolyte solutions but currently even the most advanced models cannot describe water's special properties."

Professor Georgios M. Kontogeorgis, CERE

Activity coefficients of individual ions

Another main direction is activity coefficients of individual ions (IIAC)). The topic has spurred academic controversy with some scientists claiming that ions cannot be seen in isolation. Nevertheless, PhD Researcher Martin Olsen, CERE, decided to investigate IIAC in his project:
"Several groups have reported measurements for individual ions. I am not trying to duplicate their efforts, but instead compare their findings with the thermodynamic models which we use in CERE," Martin Olsen explains, continuing:

"Studying ions is generally more complex than studying molecules. This is because while molecules are almost exclusively subject to short-range interactions, ions are able to interact over much longer distances due to their electric charge."

As his subject for the comparison, Martin Olsen chose the two ions, Na+ and Cl-, in NaCl – the most common of salts, with vast amounts of data available. Further, he chose the e-CPA model (electrolyte cubic plus association), a model largely developed in CERE.

"Overall, the comparison confirms that looking at IIAC makes sense. Still, the results are not totally as we would have expected," Martin Olsen comments.

First to include density data in e-CPA

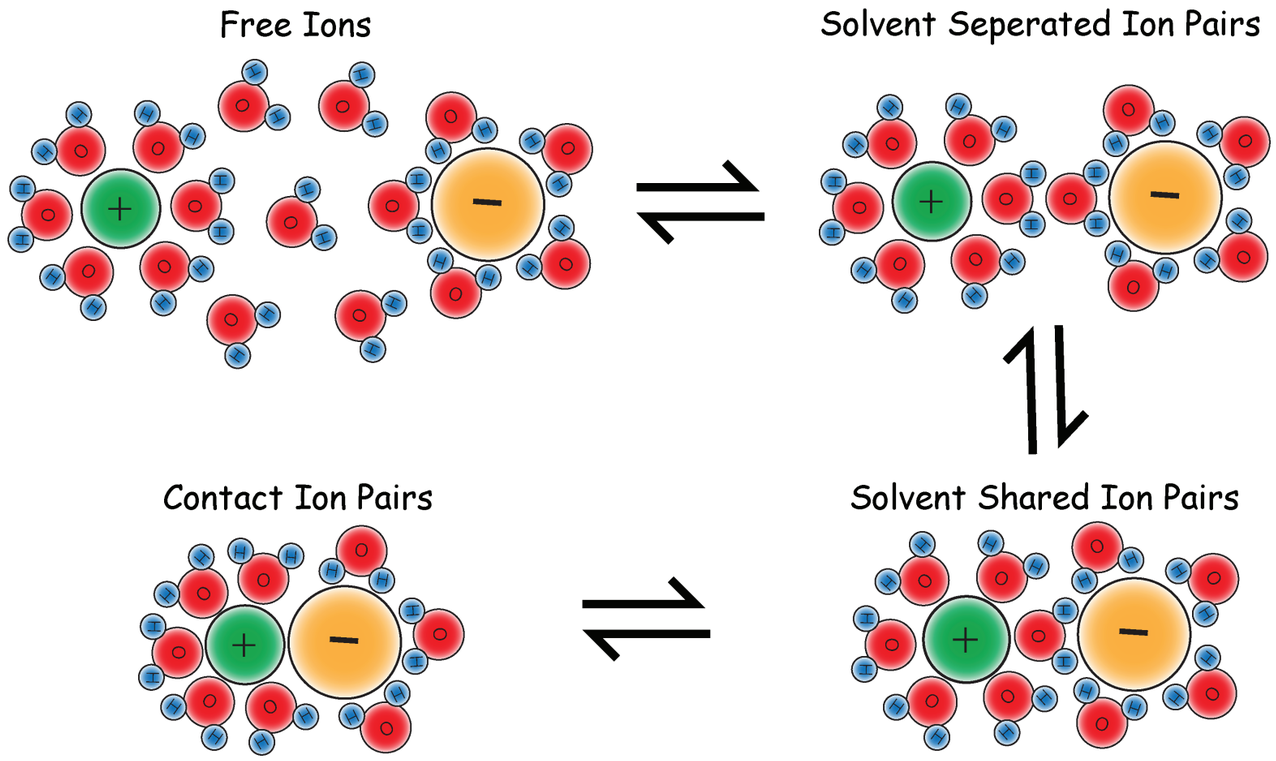
Activity coefficients are normally calculated for a salt, meaning that activity of both the anion and the cation are included. When instead the two ions are considered separately, the sum of their individual activity coefficients needs to equal the coefficient of the salt.

"This was indeed the case. However, while the sum came out as expected we would have predicted the signs of the activity coefficients of the two ions to be opposite of what was seen. This indicates that something in our understanding of electrolyte systems is still not right."

To improve understanding, Martin Olsen has included density data in parameter estimation. This is the first time for density data to be included in the e-CPA model:

"The e-CPA with density data proved to perform well, especially for prediction of the volume of the mixture. This is a key output from a thermodynamic model. Once you have an accurate prediction of your volume, several other parameters can be derived."

As for future applications, Martin Olsen says:



Ion pairs can present in a solution as free ions, contact ion pairs, solvent-shared ion pairs, and solvent-separated ion pairs. In solvent-separated ion pairs, the solvation shells of ions are intact, but ions are close enough to form a new entity in the solution. In solvent-shared ion pairs, there is one solvent molecule shared with ions. And, in contact ion pairs, both of the solvation shells break, thus there are no solvent molecules between them.

"The results do have interest for industry applications. Still, I would not expect a direct implementation. A more likely scenario is for the results to be taken up by software suppliers to improve software for parameter estimation in electrolyte systems."

Mixed solvents and gas-electrolyte systems

While possible industrial applications will be investigated at later stages, the first years of the ERC project have been dominated by basic science, Principal Investigator Georgios M. Kontogeorgis notes:

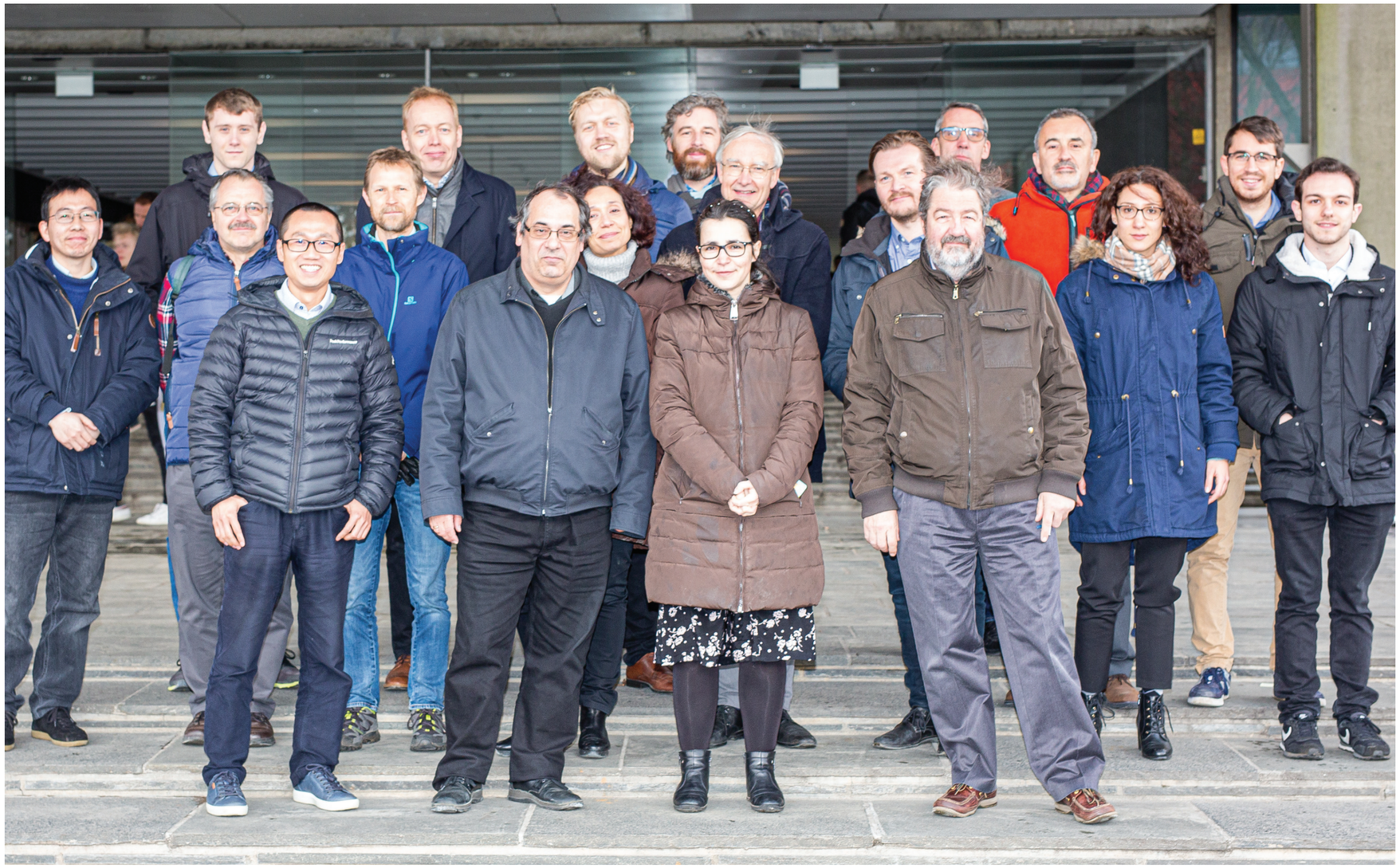
"The project aims at fundamental understanding and engineering models for electrolyte solutions. No new thermodynamic measurements will be carried out, but the vast amount of literature experimental data will be used including the in-house electrolyte database. Many data need extra checking and in-depth analysis. This is being carried out with special emphasis currently on mixed solvents and gas-electrolyte systems. The analyses and collections of data are published as part of the project in form accessible for other researchers."

With the new ground covered by the basic science in the project, Georgios M. Kontogeorgis is confident regarding the remaining years of the project:
"In many of the ERC project studies, the balance of the various terms and forces in electrolyte models are being studied. This is important as it is not at present clear which electrolyte theories are best,

exactly where they dominate and what is the role of concentration dependency of the relative permittivity. Results so far indicate small effects whether the Debye-Hückel or MSA theories are used for ion-ion interactions, results being very sensitive to ion-size and other parameters, while the relative permittivity's concentration dependency may be of importance – unclear to what extent and whether this will be covered by the parameter estimation in the models. For models only including ion-ion and ion-solvent effects, the relative permittivity and its concentration dependency play a very important role, as we have showed, but when a complete model with physical terms is considered, the situation is more complex. Studies to clarify this continue."

Testing the limits of Debye-Hückel theory

Another exiting novelty is a new PhD project on "non-primitive" electrolyte models where water will not be treated as continuum but as a real molecule interacting with ions and other molecules in the solutions.
"The comparison of "primitive" and "non-primitive" approaches is a major target of the ERC project," says Georgios M. Kontogeorgis, concluding: "In this and other projects, the limits of the 100 years old Debye-Hückel theory and the role of relative permittivity and ion-solvation are also being investigated. Lots of emphasis in many projects in 2022 on mixed solvent-electrolyte liquid-liquid equilibria, one of the greatest challenges of electrolyte thermodynamics. Finally, further projects to be launched in 2022 will involve solid-liquid equilibria and AI/ML tools applied to electrolyte systems with biomolecules."



The ERC project team at DTU for the project kick-off meeting

The ERC project

The project "New paradigm in Electrolyte Thermodynamics" is funded by the European Research Council (advanced grant scheme) and aims at both a fundamental understanding of electrolyte thermodynamics and development of engineering models in form of advanced equations of state suitable for electrolyte solutions.

Principal Investigator is Professor Georgios M. Kontogeorgis and from DTU are also participating:

- Associate Professor Xiaodong Liang (in a major role) and
- Professor Nicolas von Solms,

while Collaborators in the project in several sub-projects are:

- Professors Athanassios Panagiotopoulos (Princeton)
- Ioannis Economou, Marcelo Castier (Texas A&M, Qatar)
- Jean-Charles de Hemptinne (IFPEn)
- Dr. Bjørn Maribo-Mogensen (Hafnium Labs)

Currently five PhDs and four Postdocs are involved while an additional PhD will be employed during 2022.

The project was originally designed to run from late 2019 to September 2024. Due to COVID-19 delays, it is likely to be prolonged into 2025.

Web-site:
https://www.cere.dtu.dk/research-and-projects/framework-research-projects/new-paradigm-in-electrolyte-thermodynamics-erc-advanced-grant-project

WATER TECHNOLOGY

Michael Bache

A fresh view at water treatment

In a joint project with ferry operators Molslinjen, the CERE water research group has shown effects from electromagnetic modification of diesel fuel.

Application of a modest electromagnetic treatment will slightly change the properties of ferry diesel fuel.

"The fuel had lower viscosity, meaning it would distribute more uniformly across the combustion chamber, likely resulting in a more effective and thus less polluting combustion," reports Senior Researcher Michael Bache, CERE.

"Unfortunately, we also saw increased diesel degradation which is not acceptable. Therefore, the results cannot be applied directly in future ferry operation. In the electromagnetic treatment of water, we were able to see an increased conductivity and particle charge, this could lead to a different $CaCO_3$ scaling mechanism. Thereby our notion that electromagnetic modification does have an effect was confirmed, and we are keen to pursue this type of research further," Michael Bache comments.

Open to engaging in practical trials

For reasons which are unclear, electromagnetic treatment has become a somewhat controversial subject. While several companies manufacture equipment and claim various effects, the scientific community has often remained hesitant.

"This reservation is not unnatural, since as scientists we like not just to see an effect, but also a credible explanation for this effect," Michael Bache notes.

"However, in the case of the water molecule we have begun to understand, that the situation is much more complex than we used to think. Therefore, we should remain open to engage in practical trials involving new solutions developed by industry. Often the interaction between theoretical and practical developments is where the breakthroughs happen."

The 12-month project has been financed jointly by Molslinjen and the Maritime Fund. For the electromagnetic treatment, an apparatus from Danish company LAGUR was chosen. Through water treatment with the same equipment, the company has noted successful experiences in reducing carbonate scaling. Molslinjen wanted to see if the same was true for reduction of NOx emissions. Indeed, they did see an effect even if the electromagnetic modification was moderate – only 40 Watt and 3 Hz.

"We have been encouraged by the results and now wish to develop a new type of emitter which is dedicated for water experiments."

Senior Researcher Michael Bache, CERE.

Packing of water molecules fluctuate

Molslinjen will continue to use the LAGUR equipment for further tests.

"As for the DTU involvement, we have been encouraged by the results and now wish to develop a new type of emitter which is dedicated for water experiments," says Michael Bache.

In parallel with development of new equipment, the group continues to strive for a better understanding at the theoretical level:

"We are beginning to understand, that water is not a uniform fluid. Even at room temperature, it seems that two different phases are present. The significance of this duality – and of the interactions between these two phases – may well be huge."

The packing of the water molecules fluctuates between two packings with different densities due to the hydrogen bond network.

"It is quite possible that application of electromagnetic fields with certain frequencies may shift the balance between these two packing configurations of water. It would obviously be highly desirable to know the mechanism. Firstly, because this would be very 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 Michael Bache.

Senior Reaseacher Michael Bache

Do molecules communicate before docking?

One application under investigation by the group is drug delivery. The binding of a drug to its target protein is often described as a hand fitting into a glove. However, this docking event may be preceded by communication between the two molecules through the hydration mechanisms of the molecules. A highly ambitious project at CERE is set to investigate the phenomenon.

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

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

GEOLOGY

Thomas Guldborg Pedersen

Disclosing historic climate effects in Greenland

Icebergs floating in fiord in Greenland

Data from seismic investigations open the door to a better understanding of how the North Atlantic region will respond to current climate changes.

While oil and gas exploration in Greenland is off the table, seismic investigations conducted by the hydrocarbon industry over the most recent years may still be put to good use.

"The data give us a chance to learn how the North Atlantic geology was formed, and what has happened during historic climate changes. This understanding may help in planning for the effects of the climate changes that are happening right now," says geologist Thomas Guldborg Petersen, Associate Professor at DTU Civil Engineering and member of the CERE faculty.

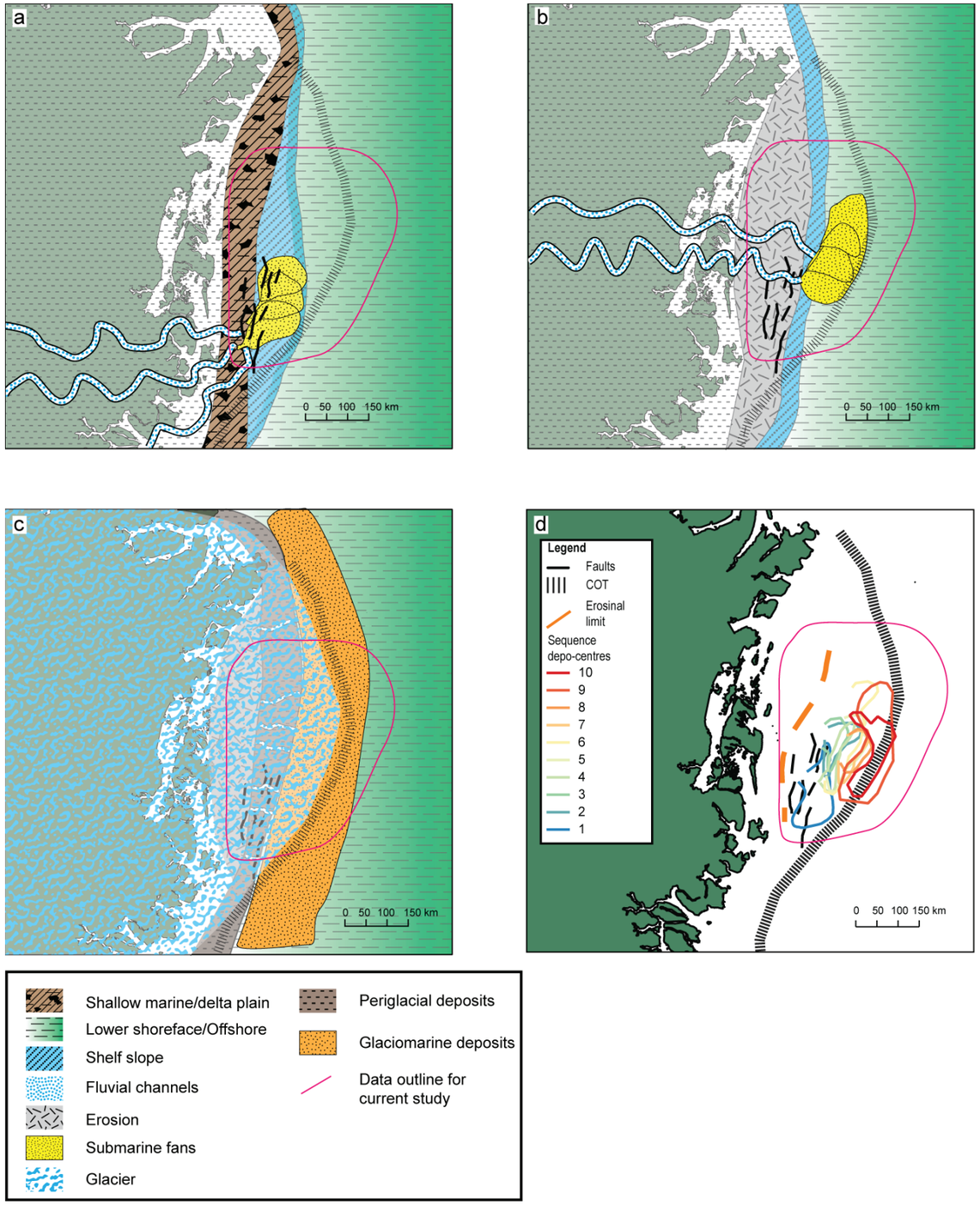
Thomas Guldborg Petersen began his academic career a little more than ten years ago, when his PhD project was financed by an energy company considering if oil and gas exploration in Greenland could become feasible. He has maintained his interest in studies of the North Atlantic geology, also after the Government of Greenland decided in July 2021 to halt all hydrocarbon exploration.

The seismic surveys from attempts to locate hydrocarbon reserves constitute a wealth of data which we could never have produced if we had relied solely on funding for independent research."

Associate Professor Thomas Guldborg Petersen, CERE.

"The seismic surveys conducted in connection with the various attempts to locate hydrocarbon reserves constitute a wealth of data which we could never have produced if we had relied solely on funding for independent research," says Thomas Guldborg Petersen, while noting that the government decision has benefitted the academic research indirectly:

"During my PhD project everything had to be kept very hush-hush. Now, with the commercial interests gone, access to seismic data is straightforward, and we are able to publish our findings in the open literature."



Geology in Northeastern Greenland and off the coast. On the third illustration (C) the extent of the ice cap at the maximum of the latest ice age is shown.

Almost virgin territory for geological drillings

Thomas Guldborg Petersen has Northeastern Greenland as his special field of interest. Few places on the planet are more difficult to access and less visited by scientific expeditions.

"In an ideal scenario we would have data from geological drillings supplementing our seismic data, but that is just not the reality. Even before the decision by the Government of Greenland, it was apparent that hydrocarbon exploration in this remote area under often harsh weather conditions would be highly challenging from a technological perspective, and financially very risky. So, no wonder that industry wasn't keen to invest in drillings that would have taken costs to another level without any certainty of ever reaching return on investment," notes Thomas Guldborg Petersen.

Still, he does have some support from drilling data, albeit indirectly. A group with the Geological Survey of Denmark and Greenland (GEUS) do parallel research based on seismic data from Western Greenland where several drillings have been carried out:

"The overall trend in the findings by the GEUS group and our group seem to be in accordance, and the fact that their findings are backed by drillings does give some level of reassurance."

Dramatic changes in the past

The seismic data produced by the hydrocarbon exploration activities shed light over the latest 1-2 million years. A time frame hard to grasp for most of us, yet a short period for a geologist as Thomas Guldborg Petersen remarks, smilingly.

During this time, the climate in Northeastern Greenland has changed dramatically many times, not least with very cold periods – known as ice ages – and warmer periods interchanging. The seismic data clearly shows that the Greenland permanent ice cap has several times been extended far into what is now the Arctic Sea.

Besides the fluctuations in temperature, also vertical and horizontal movements in the Earth's crust – so-called tectonic motions – have been at play.

"We have reason to believe that we will be able to give a much better picture of how this dynamic worked and how it led to the geology we see now in the Northern Atlantic and Arctic region," says Thomas Guldborg Petersen.

Helps estimate future climate change effects

Studies of the many dramatic climatic changes which took place in the past are likely to improve the estimates of what will happen in the region because of the current climate change, explains Thomas Guldborg Petersen:

"For instance, many would assume that as the Greenland ice cap melts, the sea water level will rise. This is however not necessarily the case locally. Firstly, the sheer body of the ice currently constitutes a significant gravitational force. So, as the ice melts away this force becomes weaker and hence the water around Greenland will not be pulled as strongly onto the shore. This may cause a lower sea water level! Secondly, the ice doesn't melt uniformly across Greenland. If we first think of a location where the ice melts away quickly, this should initiate a rise in the land below since the weight of the ice is taken off. However, various interconnectivities exist in the geology. So, when one region lifts, this may well cause another region to sink."

While this is all basic research, the practical applications are not too far away, the geologist adds:

"For instance, if you are planning a new harbor somewhere in Greenland, you really have to get these effects right. Else you risk ending up with an installation that quite soon will not match the actual sea level, and you may have wasted part of your investment."

OFFSHORE MAGNETOMETRY

Arne Døssing Andreasen

Drones assist offshore wind build-out

Unexploded bombs and mines from past wars constitute a major risk factor as the offshore wind energy sector continues to expand. Magnetic airborne surveying can reduce uncertainty.

Drone systems developed at DTU can locate so-called unexploded ordnance – bombs and mines – and other large metallic objects at the seabed. This is good news not least for the wind energy sector.

"About 90 % of the civil engineering projects currently taking place in Danish and European waters are related to establishment of wind turbine farms. Therefore, this application is our top focus," says Arne Døssing Andreasen, Senior Researcher at DTU Space, and member of the CERE faculty.

Over the past three years, the CMagTRes (Crustal Magnetism Technology & Research) group led by Arne Døssing Andreasen has developed the necessary hardware and software for a drone-based magnetic surveying system. The Royal Danish Navy EOD Services (RDN) have been a partner in the recently ended project, which was named Long-range UAV for High-Quality Magnetic Surveying (UAV-QMS,).

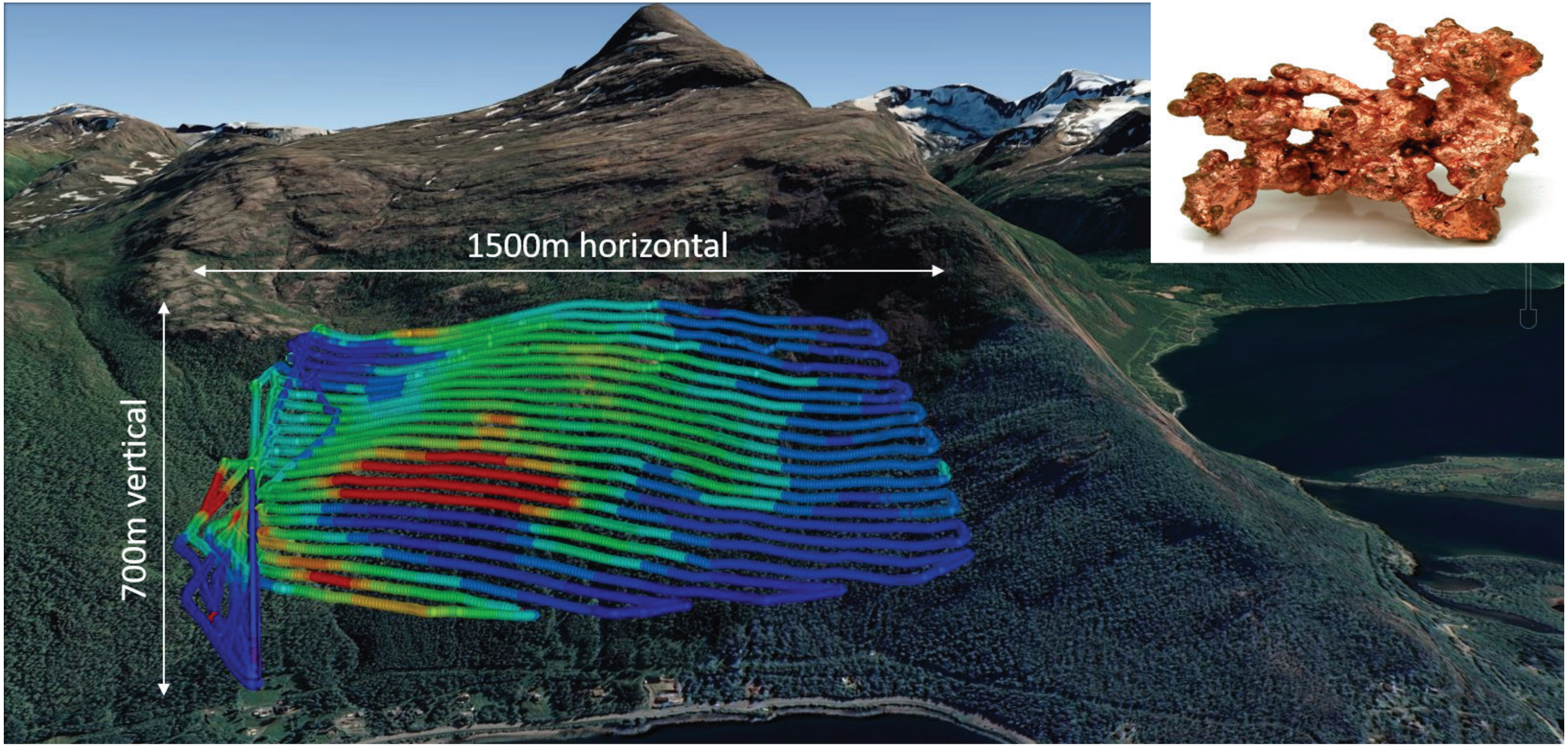
"The drone was able to locate all the metallic objects across the field, and we thus have obtained proof-of-concept."

Senior Researcher Arne Døssing Andreasen, CERE.

"The RDN have a stock of unexploded ordnance which has been cleared from Danish waters over the years. This was utilized to prepare a mock-up field for us to survey. The drone was able to locate all the metallic objects across the field, and we thus have obtained proof-of-concept. The next step will obviously be to apply the system to real industry challenges," says Arne Døssing Andreasen.

Next step: reducing uncertainty

With proof-of-concept obtained, the UAV-QMS project has served its purpose. The further development and practical implementation of the system and software takes place in a subsequent project, PROMAG (A Probabilistic and machine-learning geophysical approach for characterizing potential unexploded ordnance: A Magnetometry based study in relation to offshore wind farms in the North Sea). Here, offshore developer



Preliminary DTU drone magnetic data from a Nickel deposit in northern Norway, using a custom-developed gradiometry system. Data from this survey will be used as input for new exploration drill holes in August 2022. Carefully designed drone magnetic systems provide increased resolution and data quality at reduced cost as compared to conventional airborne systems.

Ørsted A/S is a key collaborating partner.

"We still have a number of scientific challenges to solve. Locating the positions of unexplored ordnance and other metallic objects is not enough in itself. We also want to give the depth of the object and the size. These properties are quite critical in relation to civil engineering projects, not least when estimating the costs of clearing a given area. We can supply these properties, but the interval of uncertainty is still somewhat larger than we would like it to be," explains Arne Døssing Andreasen.

The focus in the PROMAG project is drone-borne and marine magnetic data in Ørsted's database. New drone-borne high-quality data from an imitation mine field in Jægerspris and from Hornsea II offshore windfarm in United Kingdom are available to the project. Further, Ørsted A/S has provided additional data to constrain the inversion of real unexploded ordnance.

Especially relevant for shallow waters

The main objective is to create a software package that can handle large survey data sets to identify and characterize potential unexploded ordnance targets and efficiently interpret the measured anomalies by assigning a probability of it being unexploded ordnance or metal trash respectively, and further to give its size, shape, and position.

"The software package will ultimately be able to use historical unexploded ordnance data from a certain region as a training set that will allow optimization of the inversion process through machine learning," Arne Døssing Andreasen informs.

In relation to offshore wind farms, the territory of interest is much larger than the size of the farm itself. Especially the cables that take the produced power onshore will require surveying of large areas along the seabed.

"Drone surveying is especially relevant for shallow waters. In the open sea, ship-based magnetometry is generally more cost-effective. However, about 50 % of costs related to magnetic surveying in the offshore wind energy sector comes from surveying in shallow waters. It is this half of the costs that we hope to reduce," Arne Døssing Andreasen concludes.

WASTE ENGINEERING

Hariklia Gavala

Amirali Rezazadeh

Philip Fosbøl

Ioannis V. Skiadas

Kaj Thomsen

Microwaves make tricky polymer recyclable

Research assistant Amirali Rezazadeh and Research assistant Amirali Rezazadeh

PET (polyethylene terephthalate) has traditionally been difficult to recycle back to its original monomers. CERE contributes to testing and successfully developing a European innovation.

More than 500 billion plastic bottles are produced worldwide each year, and most of them are PET (polyethylene terephthalate) bottles. The figure illustrates that researchers at CERE are engaged in solving a huge societal and environmental challenge as they contribute to an innovative European research program which has managed to recycle PET.

The breakthrough stems from DEMETO (Molecular, scalable, and high-performance de-polymerization by microwave technology), a project with funding from the EU Horizon 2020 research and innovation program, and 13 European academic and industry partners (https://www.demeto.eu/).

"The monomers are of a high quality and the expected sales price should be at a level equivalent to that of monomers produced from crude oil."
Amirali Rezazadeh, Research Assistant, CERE.

Both CERE and another research center at DTU Chemical and Biochemical Engineering, PROSYS, have contributed to DEMETO.

Simulation and modelling

While our partners have designed and built the equipment – currently functional in a pilot plant in Chieti, Italy – the role of the researchers at DTU has been characterization of process streams and alternative process design, explains Amirali Rezazadeh, PhD Student in the CERE:

"We and PROSYS have contributed with our experience in process simulation and thermodynamic modelling. Having a functional technology is one thing, but as you want to take it from the lab scale to a pilot scale and in the future to full scale production, you will need to define a range of

thermodynamic parameters to be able to simulate and optimize the process to avoid ending up with excessive costs and becoming noncompetitive." Our work in CERE has contributed to the development of a simulation tool that can be used for this purpose"

PET accounts for about 18 per cent of the world's polymer production. Only PE (polyethylene), PP (polypropylene), and PVC (polyvinyl chloride) are produced in larger quantities. 60 per cent of the PET is as synthetic fibers for clothing – so-called polyester; 30 per cent is for bottles, and the remaining 10 per cent is various other applications.

Directly from bottle to monomers

One attractive property of PET for use in for example plastic bottles is stability. Since the natural degradation of the bottle is quite modest, it will be possible to recycle the bottle for the same purpose numerous times especially when a well-functioning deposit scheme is in place like in Denmark. However, the bottle will become waste material sooner or later – and this is when the stability suddenly becomes a problem.

In DEMETO, conversion of PET waste back into its composing monomers, namely ethylene glycol (MEG) and terephthalic acid (H2TP) at high enough purity for satisfying the plastics industry strict specifications, has been achieved. MEG can be sold directly for various purposes, while terephthalic acid can be the monomer building block for PET or numerous other products.

"The project idea was to develop a system so efficient that you can feed it PET waste and get the virgin monomers directly as the resulting product," says Amirali Rezazadeh.

This ambition has been fulfilled. Several steps happen on the path from PET waste to monomers.

Closing the circular economy loop

Terephthalic acid, the monomer of PolyEthylene Glycol (PET)

The core process, depolymerization, is achieved by alkaline hydrolysis through microwave treatment. Hereafter, monomers must be separated from other chemicals in the mixture, and various impurities needs to be removed, until finally the purified product is at hand.

Notably, the monomers are of a quality that fulfill market requirements and they can therefore be sold at the normal market specification.

"The monomers can be used to produce new PET bottles, closing the circular economy loop, but may also find numerous other applications for example polyester for carpets or textiles," says Amirali Rezazadeh, continuing:

"Since the microwave depolymerization runs on electric power, it will be possible to use renewable energy such as wind power or photovoltaic cells adding to the overall sustainability of the solution."
With the DEMETO funding expired and the technology becoming operational at pilot plant scale in Chieti, Italy, further development lies beyond the scope of the EU funding scheme for innovation.

"The interest of industry players of this magnitude underlines that PET recycling is both a huge environmental challenge and a significant business opportunity," Amirali Rezazadeh notes.

Price level equivalent to fossil polymers

Undoubtedly, the DTU contribution has moved the concept closer to full-scale implementation. Still, it is too early to claim commercial success, Amirali Rezazadeh underscores:

"When you have a completely new technology, you will always face some level of uncertainty regarding the degree of economy of scale you can expect. What we do know, is that the monomers are of a high quality and that the expected sales price should be at a level equivalent to that of virgin monomers produced from crude oil.

The DTU researchers involved in the DEMETO project were: Associate Professor Ioannis Skiadas (PROSYS), Associate Professors Philip L. Fosbøl, Hariklia Gavala, Kaj Thomsen, and PhD Student Amirali Rezazadeh (all from CERE).

NEWS FROM CERE

International initiative on property measurements

2021 saw the completion of an IUPAC (International Union of Pure and Applied Chemistry) project on good reporting practices for property measurements. Professor Georgios M. Kontogeorgis, CERE, contributed to the project which was led by the National Institute of Standards and Technology (NIST), USA. Also, several of the international academic and industry experts collaborating with CERE contributed.

The resulting report aims to improve experimental data quality, reproducibility, and usefulness. To this end, the report presents a series of Good Research Practice elements addressing planning, methodology, and validation of experiments.

The report is Golden Open Access and can be addressed via the CERE Consortium members website.

Securing the industrial relevance of thermodynamics

While for blockbuster movies the sequel often disappoints, the same is not true for investigations undertaken by the European Federation of Chemical Engineering. Back in 2010, the federation did a survey paper on "Industrial Requirements for Thermodynamic and Transport Properties". Ten years later the exercise was repeated to see how industry today looks at topics such as the challenges and evolution related to experimental data, models standardization and implementation, process simulation and product design, big data, machine learning, digital twins, and education in thermodynamics.

Professor Georgios M. Kontogeorgis, CERE, was leading the follow-up investigation, and several members of the CERE industry Consortium were among the survey respondents. Together, the respondents represent a broad range of companies with interests in thermodynamics – from oil to fine chemicals, gas and power, and software developers.

The resulting paper was selected as the ACS (American Chemical Society) Editor's Choice. The paper can be accessed through the CERE Consortium member website.

SPE honors Professor Erling H. Stenby

The Society of Petroleum Engineers (SPE) honors Professor Erling H. Stenby with the 2021 SPE Distinguished Achievement Award. Erling H. Stenby is the former head of CERE. For a little more than 20 years, he chaired the center and its predecessor IVC-SEP.

Besides his leading roles in CERE and IVC-SEP, Erling H. Stenby is recognized for his key role in establishment of the DTU MSc program in Petroleum Engineering. Today, the university ranks 3rd internationally in the field according to the QS World University Rankings.

Erling H. Stenby is Head of Department at DTU Chemistry. During his more than 30 years at DTU, Professor Stenby has supervised a large number of PhD students and Postdocs. His fields of expertise include phase behavior of complex systems, equations of state, computational methods, reservoir simulation, enhanced oil recovery modelling, and CO2 capture and storage. He has published more than 200 articles in peer-reviewed journals.

Further, Professor Stenby has been chairing two national Danish research councils, he is a co-founder of the spin-out Tie-Line Technology, and he is a member of the Science Council of TotalEnergies. He has served on the board of the SPE Copenhagen section and was the chairman for three years.

Professor Georgios M. Kontogeorgis new member of ATV

CERE faculty member, Professor Georgios M. Kontogeorgis, is appointed as member of the Danish Academy of Technical Sciences (ATV). The academy is an independent non-profit organization devoted to contributing to societal

debates and policy making with technical perspectives. Further, ATV works to improve the framework for science and technology research and application in Denmark.

Current areas of focus include technology for sustainability, engineering in education, and digitization of industrial production.

ATV has about 800 fellows and partner members, approximately half from academia and half from private companies. 40 new members joined the academy in 2021.

Philip L. Fosbøl joins the GEUS board

Associate Professor Philip L. Fosbøl, CERE, has been appointed to the Board of Directors of GEUS (Geological Survey of Denmark and Greenland) for the period 2021-2024. The appointment is related to his status as one of Denmark's leading experts on carbon capture.

"I am pleased to join the Board at a time where GEUS is renewing its focus on CO_2 storage," says Philip L. Fosbøl.

The Board is responsible for the general management and lays down the overall guidelines for the organization, long-term operation, and development of GEUS. Board chairman is Professor Minik Rosing, University of Copenhagen.

New chairman for the SPE student chapter

Isaac Appelquist, PhD student in CERE, is the new chairman of the SPE (Society of Petroleum Engineers) Copenhagen student chapter.

In his PhD project on oil and gas well integrity, Isaac Appelquist investigates precipitation of inorganic crystals on surfaces of wells and pipelines. By increasing understanding in this field, scaling prediction models can be improved in order to secure a more sustainable production. The study is a collaborative effort involving both CERE and the Danish Hydrocarbon Research & Technology Center (DHRTC), now Danish Offshore Technology Center (DOTC).

CERE to host waste valorization conference

In the summer of 2022, CERE and DTU Chemical and Biochemical Engineering will co-organize a major international conference within Waste and Biomass Valorization, the WasteEng ´22.

WasteEng is an international biannual conference series. The expected 300-400 participants will mainly be researchers and academics who perform research within a broad range of topic such as CO/CO_2 rich gas streams, biogas and biorefinery conversions, gasification, pyrolysis, gas emission, and remediation from incineration and combustion, catalytic processes, energy storage, and construction materials from waste. Further, several industry participants with an interest in following scientific developments are expected.

Associate Professor Hariklia N. Gavala, CERE, is Co-Chair for the event which will take place July 27-30, 2022.

Modeling course held in hybrid format

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". Following an entirely digital event in 2020 due to COVID-19 lockdowns, the course was held in a hybrid format in 2021.

"The locals were attending physically, while people who could not travel were attending via Zoom," explains Associate Professor Wei Yan, CERE.

The feedback was good as always, he continues: "Surely, all the participants wished for the event to become physical completely once COVID is over, and that is what CERE is planning for in 2022. Still, should it turn out to be necessary we are confident that we can provide online access given the experiences of online teaching and the digital materials we have produced."

Originally initiated by Professors Michael L. Michelsen and Jørgen Mollerup, since 2015 the course has been organized by Professor Georgios M. Kontogeorgis and Associate Professor Wei Yan.

Environmental topics at SPE event

Sustainable hydrocarbon production offshore was at the core of the agenda as CERE played host to a meeting of the Danish chapter of the Society of Petroleum Engineers (SPE).

Program Manager Jørgen R. Næumann of the Danish Hydrocarbon Research and Technology Center (now Danish Offshore Technology Center, DOTC) presented the Produced Water Management research program. This is the first program at (now DOTC) focused on reducing the environmental impact of oil and gas operations offshore. The goal of the program is to eliminate harmful discharges to the marine environment associated with produced water.

Christian Husum Frederiksen, Production Technology Advisor at DHRTC, presented a project on self-healing cement in the Well Production Technology program. Cement is used to isolate oil and gas wells. Also, a decommissioned well will be sealed with cement. Here, it is very important to mitigate potential leaks which could lead to oil or gas emissions. A possible solution to this challenge is self-healing cement which can repair its cracks at ambient temperature. The program aims to verify the self-healing ability at well conditions and typical offshore pumping operations.

Finally, Professor Georgios M. Kontogeorgis, CERE, offered new insights on the fundamental nature of water. Although water is familiar to everybody, its complex properties are still mysterious for the scientists. Recently, the quest for understanding water's structure has intensified. Professor Kontogeorgis summarized relevant thermodynamic theories and suggested possible implications to oil, gas, and other energy fields.

The SPE meeting was held as an online event October 27.

PhD Thesis

Hydrate swapping: Producing CH_4, storing CO_2

Jyoti Shanker Pandey, PhD.

Full title:
"Hydrate swapping for CO_2 storage and CH_4 production: Challenges and innovations."

Supervisors:
Nicolas von Solms, Alexander Shapiro.

Funded by "Independent Research Fund Denmark"

Large quantities of methane (CH_4) are stored in the form of gas hydrates in geological settings around the globe. Gas hydrates are ice-like crystalline compounds with various guest molecules surrounded by water cages. The hydrates are formed when pore water is under high pressure and low temperature. The total amount of CH_4 in these reservoirs is estimated to equal twice the known fossil fuel reserves. The advantage of injecting CO_2 into the reservoirs would be twofold: valuable CH_4 would be produced, while the CO_2 would be stored in the geological formation instead of contributing to climate change. This concept is known as hydrate swapping. In the project, a range of possible hydrate swapping methods have been examined.

Hydrate swapping is an environmentally friendly and carbon-neutral technique. Not only is CH_4 valuable, but it also actually poses a threat to the Earth's climate if left in its current geological settings. Due to rising global temperatures, CH_4 is leaking to the atmosphere, contributing further to climate change. Moreover, hydrate swapping may contribute to the stability of hydrate-bearing sediments, since CO_2 hydrates are more stable than CH_4 hydrates.

From a thermodynamics point of view, conditions for hydrate swapping are good since due to the better stability of CO_2 hydrates, CO_2 injection into CH_4 hydrates will cause spontaneous conversion from a CH_4-rich to a CO_2-rich system.

Still, despite all the potential advantages, the technique has not been applied commercially. Since the main obstacle lies in low CO_2 sweep range caused by the mass transfer barrier at the gas-liquid interface, overcoming this barrier was chosen as the focus of the project.

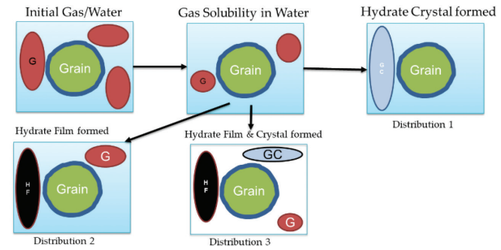
Results show that modified pore water chemistry can control the CO_2 mass transfer barrier, providing additional CH_4 recovery and CO_2 storage.

The modifications included both adding chemicals (inhibitors and promotors) in small doses, and different pressure regimes. Also, different CO_2 concentrations in the injection stream was tried – both pure and diluted. These studies were carried out using a high-pressure micromodel and a high-pressure cell. It was found that several dissociations and reforming events would occur between CH_4 and CO_2 hydrate stability pressures during slow pressure release, leading to CO_2 hydrate reformation.

The effects of hydrate saturation, residual water saturation, and reservoir temperature on recovery and storage yield with and without additives were all investigated. Further, the effect of depressurization on dissociation of CH_4 hydrates at temperatures below 0 °C was investigated but found insufficient to produce CH_4.

Finally, some new approaches to improving CH_4/CO_2 hydrate exchange were touched upon.

In conclusion, the project will hopefully contribute to the advancement of gas hydrate science and technology to recover CH_4 and store CO_2 in an environmentally friendly manner.



Hydrate morphology distribution during the hydrate formation (gas in red, water in blue and grains in green)

Ionic liquid electrolytes for battery applications

Jiahuan Tong, PhD.

Full title:
"Theory, simulation, and models for electrolyte systems with focus on Ionic Liquids".

Supervisors:
Nicolas von Solms, Suojiang Zhang, Xiaodong Liang.

The project was supported by DTU Chemical Engineering and by Beijing Key Laboratory of Ionic Liquid Clean Process, Chinese Academy of Sciences.

High-performance batteries play a vital role in meeting the needs of electric vehicles, large energy storage equipment, and other industries. Lithium-ion batteries dominate the market due to high voltage, high specific energy, and long cycle life. However, most lithium-ion battery electrolytes use lithium salts dissolved in organic solvents. These mixes are generally toxic, volatile, and have low ignition points which cause environmental and safety issues. Recently have Ionic Liquids (ILs) emerged as safer alternatives. The project investigates the use of ILs in battery electrolytes.

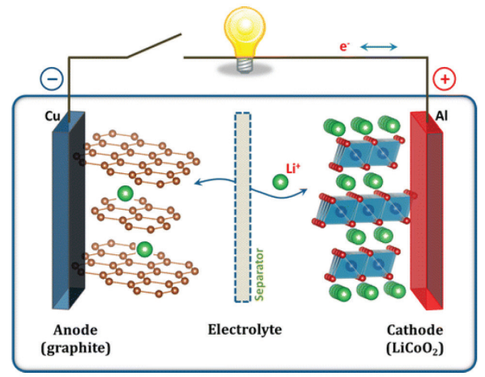
ILs are salts but unlike the common perception of salts, they are liquid at room temperature. Since the vapor pressure in IL is extremely low, close to negligible, the risk of losing IL due to vaporization is minimal. Importantly, IL solvents can be designed for the specific purpose. However, some properties related to the use of IL electrolytes remain unsolved, including the solvation effect, the kinetic behavior, and the mechanism of lithium-ion transport.

In the project, two organic solvents and four IL solvents were computationally investigated for the high concentration lithium electrolytes, 2mol/L lithium bis(trifluoromethylsulfonyl) imide (LiTFSI).

The simulations show that the IL solvent electrolytes exhibit higher density and viscosity, larger self-diffusion coefficient, and conductivity than the organic solvent electrolytes. Moreover, [C4mim][BF4] was shown to have the highest conductivity among the IL-based electrolytes. Microstructure studies revealed that the organic solvents restrict the free movement of the ions and reduce the conductivity of the electrolytes.

Studies showed the density and viscosity of IL electrolytes and the transfer of lithium ions to increase with the LiTFSI concentration. Structural analysis indicated strong bidentate and monodentate coordination between Li+ and anion of all IL electrolytes. More importantly, the existence of the ion cluster [Li[anion]x] (x-1)- in IL electrolytes was found, and the cluster became more compact as the LiTFSI concentration increased.

Further microstructure studies showed that negative lithium transference number and negative effective charge exist, which is caused by strong interactions in IL electrolytes with different lithium concentrations. Due to the consideration of ion dependence, the negative lithium transference number behavior fundamentally deviates from the apparent transference number obtained using the self-diffusion coefficient analysis. In addition, the calculation of the effective lithium-ion charge shows that the lithium-containing clusters in the IL electrolytes are always negatively charged in a very wide range of concentrations. This indicates that the lithium ions in the IL electrolytes are transferred by the lithium ion-anion charged cluster transfer mechanism. This discovery appears to be of great significance to the understanding of the lithium-ion transfer mechanism in lithium-ion batteries.



Schematic illustration of the first Li-ion battery (LiCoO2/Li+ electrolyte/graphite)

Production of methane from natural gas hydrates

Meng Shi, PhD.

Full title:
"Study of the application and mechanism of enhanced methane recovery from hydrate."

Supervisors:
Nicolas von Solms
John M. Woodley

The project was funded by DTU and by the China Scholarship Council.

Natural gas hydrates (NGH), the main component of which is methane (CH_4), have received growing attention in the global energy system. Large amounts of NGH resources exist in permafrost and offshore in continental margin zones. The global methane reserves in NGH are estimated to be equivalent of at least half the total offshore oil and gas resources. In the project, potential technologies for production of methane from NGH with storage of CO_2 as an added benefit are investigated.

Gas hydrates consist of water molecules as the host and gas molecules as the guest. Under the right circumstances, one type of guest gas molecules – in this case CH_4 – can be substituted by another. In the project, CO_2 is used as the substituent molecule. The motivation is twofold. Firstly, the thermodynamic properties of CO_2 are well suited for replacing CH_4 in the hydrates. Secondly, storage of CO_2 is desirable as a way of mitigating climate change.

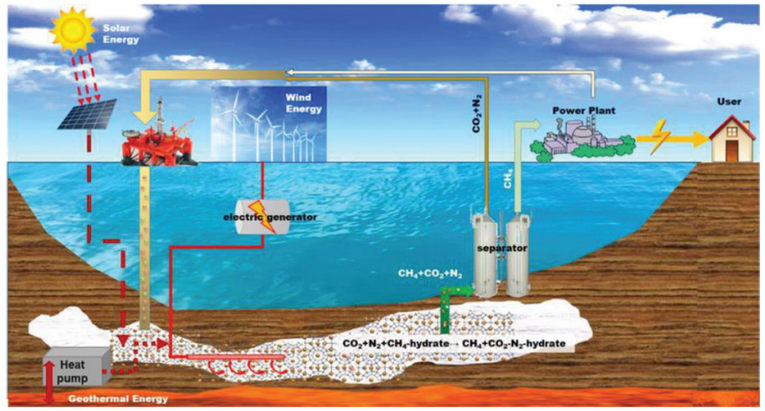
Three groups of spherical methane hydrate samples with variant diameters of 11 mm, 17 mm, and 22 mm were prepared to simulate NGH particles in lab experiments. The results show that the effect of depressurization is significant on the methane recovery ratio, while the effect of the surface-area-to-mass ratio is less significant. During the hydrate decomposition process, the methane production rate increases with increasing operating pressure and surface-area-to-mass ratio.

The recovery efficiency was investigated using combined three-stage depressurization assisted with CO_2-enriched air injection. Injecting CO_2-enriched air promoted the performance of gas hydrate production with up to a 74.4 % recovery ratio compared with injecting air. For the first time, a novel multilayer hydrate cap mechanism is proposed to describe the improved efficiency during the replacement-depressurization process. The results from this study are beneficial for future optimization of operating conditions to maximize efficiency and develop planning for NGH resources.

Further, the effect of hydrate structural properties on the decomposition process was theoretically investigated. A sudden decrease in potential energy was observed for one-step depressurization during simulation times ranging from 1.5 ns to 3 ns. F4 order parameter investigation confirmed a tendency for regeneration of hydrates during this period. The diffusion coefficient can also be improved by an increase in temperature.

Multi-step depressurization compensates for energy loss by including the released methane molecules dissolved in the liquid water phase, thus breaking the tendency for hydrate reformation during decomposition. The application of multi-step depressurization in molecular simulation can provide significant insights for on-field hydrate resource exploitation and help to understand the mechanisms behind hydrate production at the molecular scale.

In conclusion, the results from the project provide an improved understanding of methane hydrate production driven by depressurization, CO_2 replacement, at its combined performance.



Concept of a future combined system for gas hydrate exploitation

Fluid distribution in petroleum reservoirs

Hadise Baghooee, PhD.
Currently with Haldor Topsøe A/S.

Full title: "Characterization of the fluid distribution in petroleum reservoirs."

Supervisors:
Alexander Shapiro
Charlotte Lassen
Wei Yan.

Funding was providing by the Danish Hydrocarbon Research and Technology Centre (DHRTC).

Especially in tight formations, the distribution of hydrocarbons is not necessarily uniform across a reservoir. Non-uniform distribution is a challenging factor when planning the reservoir development. Further, it can be difficult to obtain relevant samples not least from tight reservoirs such as the Valdemar field in the Danish part of the North Sea. In the project, models for characterization of the fluid distribution in petroleum reservoirs were developed and some aspects of hydrocarbon mixture distribution in the Valdemar field analyzed.

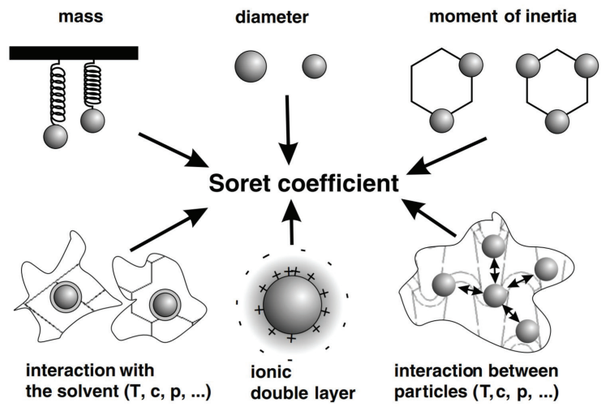
Indefiniteness in the lateral variation of the hydrocarbon composition is an important factor affecting the prospective development of the Valdemar field and other Lower Cretaceous fields in the North Sea. Some observations have been puzzling. Moreover, it is challenging to obtain representative fluid samples firstly due to the low permeability of the reservoir rock and secondly since the fluids are near saturation. Each sample should undergo a thorough thermodynamic consistency test. Both gravity and temperature variation contribute to differences in petroleum composition. Thermo-diffusion is the governing phenomenon determining the contribution of the geothermal gradient (variation of the temperature along the reservoir depth). Here, transport coefficients like diffusion and thermo-diffusion are the key parameters.

In the project, a unified thermodynamic model for the diffusion and thermo-diffusion was developed. By introducing new emission functions and penetration lengths, some well-known expressions for diffusion and thermo-diffusion coefficients in binary mixtures were matched. The model was verified by comparison with the experimental diffusion and thermo-diffusion data for binary mixtures.

Moreover, the effect of non-equilibrium thermodynamic models was applied to calculate the compositional gradients under the varying temperature. To determine the variations in pressure and composition with depth, a model based on the principles of irreversible thermodynamics was developed. The distribution of hydrocarbons in a reservoir was described based on the Onsager relationships where pressure, chemical potentials, and thermal gradient are linked. A computational algorithm accounting for the non-ideality of the mixture, characterization, and phase transition was developed. The model and the computational procedure were validated by comparison with case data. I was shown that the model can predict the fluid distributions with depth with no or a minimum of adjustable parameters.

Based on representative samples from the Valdemar reservoir, it was illustrated how a depth gradient analysis can help in understanding fluid communication between the different points in the reservoir.

An important practical outcome from the project is the reduction of indefiniteness in the fluid characterization of tight petroleum reservoirs in the North Sea, improving their development prospects.



The main features determining thermodiffusion behavior

Prediction of the relative oil permeability in tight chalk

Wael Fadi Al-Masri, PhD

Full title:
"Gas liberation in tight porous media".

Supervisors:
Alexander Shapiro
Wei Yan.

Funding: Danish Hydrocarbon Research and Technology Centre (DHRTC) as part of the Lower Cretaceous program. The Danish Underground Consortium has kindly provided the core samples used in the project.

While hydrocarbon exploration in the Danish part of the North Sea to date has been concentrated on the younger Upper Cretaceous layers, also the Lower Cretaceous layers contain substantial oil and gas reserves. However, these deep layers are dominated by extremely low-permeable chalk, and exploration is complex. 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. It has been hypothesized that this effect may be caused by gas bubbles appearing in the oil as the reservoir pressure drops with oil production. When oil reservoirs are developed, the pressure decreases. If pressure drops below the so-called bubble-point, gas is liberated from the oil. The liberated gas bubbles plug the porous space of the reservoir and create additional resistance to the oil flow. This the so-called Jamin effect has been long known in medicine, where a bubble of the air, eventually appearing in the blood because of inaccurate injection might stop the blood flow and result in infarction. As applied to petroleum, this means that the appearing gas bubbles may plug capillaries of the porous reservoir rock and prevent oil from moving. The effective (relative) permeability to oil may thus decrease as a result of gas liberation. In the project, this phenomenon has been studied experimentally, and a model for predicting oil relative permeability in such situations has been developed.

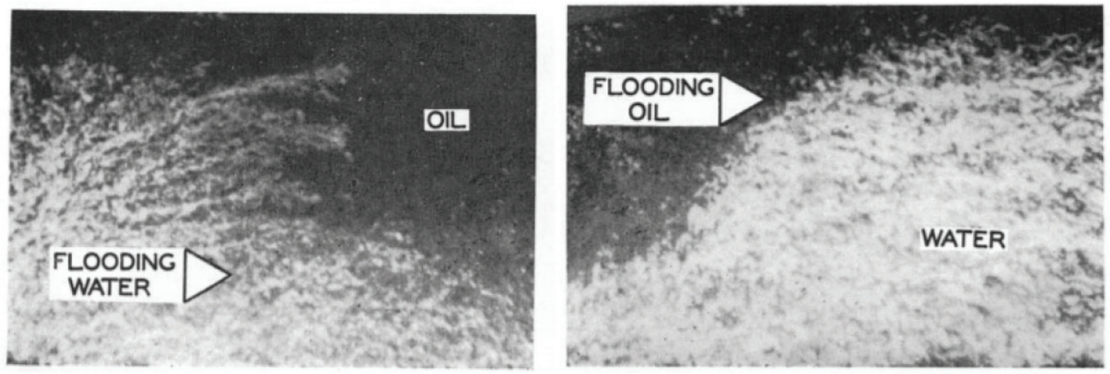
In the project, a new method to measure oil relative permeability and critical gas for oil-gas systems under depressurization was developed. The oil relative permeability is measured in the presence of immobile gas. The amount of liberated gas is determined by application of the X-ray computer tomography. The novelty is the ability of the proposed method to measure the relative permeability outside the active saturation region.

Further, a model was derived for predicting the relative permeabilities under two-phase flows in porous media. The dependencies for the relative permeabilities on the saturation were derived based on a pore-level model of the porous medium, represented as a capillary network. The distribution of bubbles of droplets in the network is computed statistically using a method adapted from statistical physics in combination with percolation theory.

The model makes it possible to evaluate relative permeabilities based on a relatively small number of parameters. These parameters may be found either from the microstructure of the porous medium or from using one core sample to predict the rest.

Comparing model predictions with the experimental data has assured the soundness of the model, which was later applied for the reservoir simulation.

The model was derived for the purpose of predicting oil relative permeability for the case of bubble formation in an oil reservoir when the pressure falls below the bubble point. However, the project has revealed that the model can also be used in the case of condensation and droplet precipitation in a gas-condensate reservoir.



Visualization of the channeling effect during water and oil flooding experiment (Chatenever and Calhoun, 1952).
The pictures illustrate the individual paths created by each fluid.

Computer-aided design of organic coatings

Markus Jannert Enekvist, PhD.

Full title: "Computer-aided product design of organic coatings".

Supervisors: Georgios M. Kontogeorgis, Xiaodong Liang, Kim Dam-Johansen, Xiangping Zhang.

The project was a part of the Hempel Foundation Coatings Science and Technology Centre (CoaST). Funding was provided by the Hempel Foundation and the Sino-Danish Center.

Current formulation practices in paint and coating development are based on a time-intensive iterative process of trial-and-error. An emerging alternative is advanced product formulation, where products with the desired characteristics are designed through a combination of computer-aided tools, experimentation and experience. This approach can not only reduce development time, but also limit the use of substitute chemicals with a detrimental effect to nature or human health. In the project, methods for computer-aided coating design have been developed.

A key challenge in coating design is the wide range of components including pigments, polymers, solvents, and additives. With a solvent fraction of up to 50 % by volume, efforts are made to reduce the environmental footprint and usage of organic solvents. Still, it remains a complex challenge to ensure that improved sustainability does not come at the cost of poorer technical performance. Computer-aided product design consists of a combination of computational tools, algorithms, large databases and predictive methods for the estimation of different product properties. The key concept is to reduce the overall highly complex task to individual tasks which each requires specific inputs and tools.

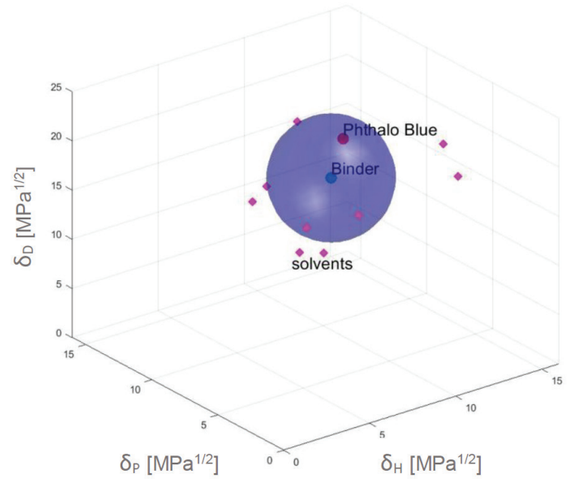
In the project, new property estimation methods for organic pigments have been developed for the partial solubility parameters while systematic methodologies for solvent selection for organic coating formulations have been proposed and tested.
Firstly, property models were developed for the dispersion, polar, and hydrogen-bonding partial solubility parameters. New groups suitable for colorants were added based on conjugation theory, to improve the predictive power.

Secondly, a systematic framework was proposed consisting of databases, methods, and tools for the design of paint formulations and their solvents. The framework expands upon established algorithms and software and includes several screening steps in increasing order of computational difficulty. The early steps test the phase stability and linear requirements of the solvent mixtures. Later stages apply requirements such as RED, flash points, and evaporation rates. The final level provides environmental and health-based properties.

Lastly, the viability of extending computer-aided methods to the selection of ingredients for non-solvent-based coating systems was investigated.

The computer-aided product design used throughout the project could be integrated in formulation software currently used by industry. Features like phase stability and component compatibility would be a useful addition to traditional features including density, pigment volume concentration, and solids contents.

In conclusion, application of the tools developed in the project can provide a formulator with a more accurate starting point when developing new products, and focus experiments on a selected number of screened ingredients from a potentially large search space.



A three-dimensional illustration of the Hansen Solubility Parameters of a binder, an organic pigment, and several solvents. The blue sphere represents a Relative Energy Difference of unity.

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Caroline Grunnet Rudbeck, DTU Chemical Engineering

Conference contributions & invited speakers

MARCH

Virtual GHGT-15, Abu Dhabi, 15-18 March 2021

Randi Neerup, Carolina. F. Murcia, Isaac A. Løge, Kaj Thomsen, Philip L. Fosbøl, "FeCO3 mineralization and solubility - a guiding factor CO2 corrosion and storage", Virtual GHGT-15, Abu Dhabi, 15-18 March 2021 (Oral presentation)

Randi Neerup, Kenny Ståhl, Philip L. Fosbøl, "Amine polymerization is a new observed molecular behavior in CO2 capture", Virtual GHGT-15, Abu Dhabi, March 15-18 2021. (Poster presentation)

Wentao Gong, Rik Timmermans, Eryk Remiezowicz, Philip L. Fosbøl, Nicolas von Solms, "Design and Analysis of Novel CO2 Conditioning Processes in the 3D Project", Virtual GHGT-15, Abu Dhabi, 15-18 March 2021 (Oral presentation)

Lucas F. F. Corrêa, Philip L. Fosbøl, Indira Jayaweera, Palitha Jayaweera, Kaj Thomsen, "New Apparatus for CO2 Solubility Measurements From Total Pressure-composition Data", Virtual GHGT-15, Abu Dhabi, 15-18 March 2021 (Oral presentation)

Sai H. B. Vinjarapu, Laurette Madelaine, Nicolas von Solms, Philip L. Fosbøl, "New Technologies for Energy Reduction in Biogas Upgrading", Virtual GHGT-15, Abu Dhabi, March 15-18, 2021 (Poster presentation)

DESY Centre for Molecular Water Science (CMWS) DAYS 2021, Hamburg, Germany, 25 March 2021

Michael Bache "Study of electromagnetic communication between chiral drug molecules and its receptor in water", DESY Centre for Molecular Water Science (CMWS) DAYS 2021, Hamburg, Germany, 25 March 2021 (Oral presentation)

Thermal Analysis and Calorimetry - TAC 2021 - Virtual conference, Huddersfield, United Kingdom, 29-30 March 2021

Jyoti Shanker Pandey, "Enhanced CH4 Hydrate Formation using Hybrid MOF plus Promoter System", Thermal Analysis and Calorimetry - TAC 2021 - Virtual conference , Huddersfield, United Kingdom, 29-30 March 2021 (Oral presentation)

MAY

DHRTC Young Researcher Day, (online) 7th May 2021

Sindhu Vudayagiri, Johannes Liljenhjerte, Nicolas von Solms, Jens Vinge Nygaard, "Extended Reach Interventions", DHRTC Young Researchers Day, (online) 7 May 2021 (Oral presentation)

Working Party on Thermodynamics and Transport properties, Toulouse, France, 19 May 2021

Georgios M. Kontogeorgis, "Thermodynamic modeling of electrolyte solutions using the Debye-Hückel theory", EFCE Spotlight Talks (Online), (Oral presentation)

8th International Conference on Engineering for Waste and Biomass Valorisation, Virtual, Guelph, Ontario, Canada, Online 31 May - 4 June, 2021

Antonio Grimalt-Alemany, Konstantinos Asimakopoulos, Christina Etler, Ioannis V. Skiadas, Hariklia N. Gavala, "ORP control for boosting ethanol productivity and dynamics of redox cofactor NADH/NAD+ under oxidative stress", 8th International Conference on Engineering for Waste and Biomass Valorisation, Virtual, 31 May – 4 June 2021 (Oral presentation)

Hariklia N. Gavala, "Biotransformations of syngas: A sustainable way forward", 8th International Conference on Engineering for Waste and Biomass Valorization, Virtual, Guelph, Canada, 31 May-4 June (Keynote talk)

Amirali Rezazadeh, Antonios Melas, Hariklia N. Gavala, Kaj Thomsen, Philip L. Fosbøl, Ioannis V. Skiadas, "DEMETO: Sustainable chemical recycling of PET and Polyester", 8th International Conference on Engineering for Waste and Biomass Valorization, Virtual, Guelph, Canada, 31 May-4 June (Oral Flash presentation)

Konstantinos Asimakopoulos, Antonio A. Grimalt-Alemany, Hariklia N. Gavala, Ioannis V. Skiadas, "Syngas biomethanation in trickle bed reactors by anaerobic mixed microbial consortia", 8th International Conference on Engineering for Waste and Biomass Valorization, Virtual, Guelph, Canada, 31 May-4 June (Oral Flash presentation)

InterPore 2021 (Virtual conference): 13th Annual Meeting - Online Conference, Berlin, Germany, 31 May-4 June 2021

Jyoti Shanker Pandey, "Pore Scale Visualization of CH4-CO2 Mixed Hydrates Phase Transitions During Stepwise Depressurization" InterPore 2021 (Virtual conference): 13th Annual Meeting - Online Conference, Berlin, Germany, 31st May - 4th June 2021 (Oral presentation)

Jyoti Shanker Pandey, "MOFs based CH4 Hydrate Formation and Self-Preservation", InterPore 2021(Virtual conference): 13th Annual Meeting - Online Conference, Berlin, Germany, 31 May - 4 June 2021 (Poster presentation)

JUNE

The Biot-Bazant conference, online, Illinois, Texas, USA, June 1-3, 2021

Tobias Orlander, Ida L. Fabricius, "Including temperature in the effective stress equation - a case study from the deep North Sea basin", The Biot-Bazant conference, online, Illinois, Texas, USA, June 1-3, 2021 (Oral presentation)

Ida L. Fabricius, E. Omdal, "Elastic strain of chalk due to oil production", The Biot-Bazant conference, online, Illinois, Texas, USA, June 1-3, 2021 (Oral presentation)

Leonardo T.P. Meireles, C. Lyu, Ida L. Fabricius, T. Ingeman-Nielsen, "Towards a rock physical model for fine grained permafrost: Insights from velocity and NMR measurements", The Biot-Bazant conference, online, Illinois, Texas, USA, June 1-3, 2021 (Oral presentation)

Tobias Orlander, Ida L. Fabricius "Including temperature in the effective stress equation – case study from the deep North Sea basin", The Biot-Bazant conference, online, Illinois, Texas, USA, June 1-3, 2021 (Oral presentation)

Ermis Proestakis, Leonardo T.P. Meireles, Ida L. Fabricius, "Detecting shear wave arrival in highly porous chalk", The Biot-Bazant conference, online, Illinois, Texas, USA, June 1-3, 2021 (Oral presentation)

TCCS-11 virtual conference, Trondheim, Norway, 22-23 June 2021

Fernando Medeiros, Erling H. Stenby, Wei Yan, "The Influence of Aquifer Geochemistry on Salt Precipitation During CO2 Injection: Insights from 1D Simulations Using the RAND Algorithm" (Oral)

Sai H. B. Vinjarapu, Teresa R. Muniz, Philip L. Fosbøl, "Heat of absorption of CO2 in novel energy reducing solvents for biogas upgrading", TCCS-11 Virtual Conference, Trondheim, Norway, 22-23 June 2021 (Oral presentation)

Randi Neerup, Caroline G. Rudbeck, Isaac A. Løge, Philip L. Fosbøl, "CO2 impact on FeCO3 corrosion product", TCCC-11 virtual conference, Trondheim, Norway, 22-23 June 2021 (Oral presentation)

Isaac L. Appelquist, Randi Neerup, Philip L. Fosbøl, "Synthesis properties of FECO3: Understanding the underground reactiverock", TCCC-11 virtual conference, Trondheim, Norway, 22-23 June 2021 (Poster presentation)

Goldschmidt, online, Lyon, France 2021, 4-9 June, 2021

Randi Neerup, R., *Isaac L. Appelquist, Philip L. Fosbøl, "Thermal properties of a CO2 sorbent and its possible degradation pathways", Goldschmidt, online, Lyon, France, 4-9 June, 2021 (Oral presentation)

Isaac L. Appelquist, Randi Neerup, Philip L. Fosbøl, "Grain and crystalline domain properties of a potential CO2 storage unit", Goldschmidt, online, Lyon, France 2021, 4-9 June (Oral presentation)

Isaac L. Appelquist, Philip L. Fosbøl, Randi Neerup, "Tracking the temporal evolution of Ostwald ripening in CaCO3 crystals, related to phenomena observed under CO2 storage", Goldschmidt, online, Lyon, France 4-9 June, 2021 (Oral presentation)

JULY

The 31st European Symposium on Applied Thermodynamics, ESAT 2021 virtual conference, Paris, France, 3-7 July 2021

Fernando Medeiros, Erling H. Stenby, Wei Yan"RAND-based Geochemical Calculation Algorithms for CO2 Sequestration", The 31st European Symposium on Applied Thermodynamics, ESAT 2021 virtual conference, Paris, France, 3-7 July 2021 (Oral presentation)

Fernando Medeiros, Erling H. Stenby, Wei Yan, "State-Function Based Flash Specifications for Open Systems in the Absence or Presence of Chemical Reactions", The 31st European Symposium on Applied Thermodynamics, ESAT 2021 virtual conference, Paris, France, 3-7 July 2021 (Poster presentation)

Fernando Medeiros, Erling H. Stenby, Wei Yan, "Application of State Function-Based Phase Equilibrium Algorithms to Open Geochemical Systems", The 31st European Symposium on Applied Thermodynamics, ESAT 2021 virtual conference, Paris, France, 3-7 July 2021 (Oral presentation)

Yibo Yang, Teresa Regueira, Erling H. Stenby, Wei Yan, "Measurement and modeling of high-pressure diffusion coefficients of methane in pure hydrocarbons and reservoir fluids", The 31st European Symposium on Applied Thermodynamics, ESAT 2021 virtual conference, Paris, France, 3-7 July 2021 (Poster presentation)

Wei Yan, Christos Tsanas, Erling H. Stenby, Even Solbraa, "Comparison of engineering models in describing high-pressure properties of natural gas related systems", The 31st European Symposium on Applied Thermodynamics, ESAT 2021 virtual conference, Paris, France, 3-7 July 2021 (Poster)

Daniel Qvistgaard, "New Association Schemes for Tri-Ethylene Glycol (TEG)", The 31st European Symposium on Applied Thermodynamics, ESAT 2021 virtual conference, Paris, France, 3-7 July 2021 (Oral presentation)

Evangelos Tsochantaris, Xiaodong Liang, Georgios M. Kontogeorgis, "Application and evaluation of CPA and PC-SAFT on water for different sets of parameters", The 31st European Symposium on Applied Thermodynamics, ESAT 2021 virtual conference, Paris, France, 3-7 July 2021 (Poster presentation)

Georgios M. Kontogeorgis, "Industrial requirements for thermodynamic and transport properties -2020", The 31st European Symposium on Applied Thermodynamics, ESAT 2021 virtual conference, Paris, France, 3-7 July 2021 (Oral presentation)

F. Yang, J. C. de Hemptinne, Georgios M. Kontogeorgis, "The (water + alcohol + alkali halide) mixed-solvent electrolyte systems: Data status and consistency analysis", The 31st European Symposium on Applied Thermodynamics, ESAT 2021 virtual conference, Paris, France, 3-7 July 2021 (Poster presentation)

Nefeli Novak, Georgios M. Kontogeorgis, Marcelo Castier, Ioannis G. Economou, "Modeling of water-hydrocarbon phase equilibria with the SAFT-VR Mie equation of state", The 31st European Symposium on Applied Thermodynamics, ESAT 2021 virtual conference, Paris, France, 3-7 July 2021 (Oral presentation)

Xiaodong Liang, Georgios M. Kontogeorgis, "On the parameters in the Debye-Hückel theory", The 31st European Symposium on Applied Thermodynamics, ESAT 2021 virtual conference, Paris, France, 3-7 July 2021 (Oral presentation)

Xiaodong Liang, Georgios M. Kontogeorgis, "Critical point of associating fluids from the CPA equation of state", The 31st European Symposium on Applied Thermodynamics, ESAT 2021 virtual conference, Paris, France, 3-7 July 2021 (Poster presentation)

ISSP-19 virtual conference, Los Alamos, New Mexico, USA, 11-16 July 2021

Fernando Medeiros, Erling H. Stenby, Wei Yan, "Rand-based Algorithms Applied to Electrolyte Mixtures: Analysis of Open Systems at Specified Fugacities and Closed Systems at Saturation Conditions", ISSP-19 virtual conference, Los Alamos, New Mexico, USA, 11-16 July 2021 (Poster presentation)

Lucas F. F. Corrêa, Kaj Thomsen, Philip L. Fosbøl, "Measurement of CO2 Solubility in Mixed Solvents", ISSP-19 virtual conference, Los Alamos, New Mexico, USA, 12-16 July 2021 (Oral presentation)

11th Liquid Matter Conference 2020/2021, Virtual, Prague, Czech Republic, 18-23 July 2021

Aswin Vinod Muthachikavil, Baoliang Peng, Georgios M. Kontogeorgis, Xiaodong Liang, "Influence of Hydrogen bonds on the tetrahedral environments in liquid water", 11th Liquid Matter Conference 2020/2021, Virtual, Prague, Czech Republic, 18-23 July 2021 (Poster presentation)

SEPTEMBER

The 9th international symposium on Molecular Thermodynamics and Molecular Simulation (MTMS ´21), virtual, Akiu hot springs, Sendai, Japan., 7-9 September 2021

Georgios M. Kontogeorgis, "How can molecular concepts help in the development of more predictive advanced equations of state", The 9th international symposium on Molecular Thermodynamics and Molecular Simulation (MTMS ´21), virtual, Akiu hot springs, Sendai, Japan., 7-9 September 2021 (Plenary talk)

4th European Conference on Metal Organic Frameworks and Porous Polymers (EuroMOF2021), Virtual event, Krakóv, Poland, 13-15 September 2021

Jyoti Shanker Pandey, "CO2 Storage in Gas Hydrate Phase using MOF based Hybrid System", 4th European Conference on Metal Organic Frameworks and Porous Polymers (EuroMOF2021), Virtual event, Krakóv, Poland, 13-15 September 2021 (Poster presentation)

SPE Annual Technical Conference and Exhibition (ATCE), Dubai, United Arab Emirates, 21-23 September 2021

Yibo Yang, Teresa Regueira, Hilario Martin Rodriguez, Alexander Shapiro, Erling H. Stenby, Wei Yan, "Determination of methane diffusion coefficients in live oils for tight reservoirs at high pressures", SPE Annual Technical conference and Exhibition, Dubai, UAE, 21-23 September, 2021 (Oral presentation)

13th Conference of the European Pediatric Formulation Initiative (EuPFI) 'Formulating better medicines for children', Virtual, 22-23 September 2021

Olivia A. Perederic, Leonie Wagner, Marie Pepelnjak, Carsten Timpe, Patrick M. Piccione, Georgios M. Kontogeorgis, "Modelling endeavors for bitter taste assessment of chemicals - an overview" , 13th Conference of the European Pediatric Formulation Initiative (EuPFI) 'Formulating better medicines for children', Virtual, 22-23 September 2021 (Poster presentation)

7th International Symposium on Gasification and its Applications, Nancy, France, online 27-30 September

Hariklia N. Gavala, "Syngas biomethanation: an alternative way to energy storage", 7th International Symposium on Gasification and its Applications, Nancy, France, online 27-30 September (Plenary talk)

NOVEMBER

AIChE 2021 Annual Meeting, Boston, Massachusetts, USA, 7-11 November 2021

Fernando Medeiros, Erling H. Stenby, Wei Yan, "Saturation Point Calculations in Reactive Systems Based on the RAND Method", AIChE 2021 Annual Meeting, Boston, Massachussetts, USA, 7-11 November 2021, (Oral video presentation)

Jyoti Shanker Pandey, "Electrical Resistance Measurement during CH4-CO2 Mixed Hydrate Formation and Dissociation in Sandstone", AIChE 2021 Annual Meeting, Boston, Massachusetts, USA, 7-11 November 2021, (Oral video presentation)

Isaac L. Appelquist, Christopher G. Klingaa, Judith Cabello, Marcus Craig, Randi Neerup, Philip L. Fosbøl, "The Temperature Dependence of BaSO4 Surface Precipitation Kinetics", AIChE 2021 Online Annual, Boston, Massachusetts, USA, 7-11 November 2021 (Oral video presentation)

Sai H. B. Vinjarapu, Philip L. Fosbøl, "Heat of absorption of CO2 in novel solvents for biogas upgrading", AIChE 2021 Annual Meeting, Boston, Massachussetts, USA, 7-11 November 2021 (Oral video presentation)

DHRTC Technology Conference 2021: Oil and Gas R&D towards 2050 - supporting the energy transition, Kolding, Denmark, 16-17 November 2021

Leonardo T.P. Meireles, Ida L. Fabricius, "Strain modeling in a chalk reservoir", DHRTC Technology Conference 2021: Oil and Gas R&D towards 2050 - supporting the energy transition, Kolding, Denmark, 16-17 November 2021, (Poster presentation)

Ermis Proestakis, Leonardo T.P. Meireles, Ida L. Fabricius, "Are diatomites threatening the stability of closed wells? The possibility of the Lark Formation transmitting hydrocarbons into penetrating wells", DHRTC Technology Conference 2021: Oil and Gas R&D towards 2050 - supporting the energy transition, Kolding, Denmark, 16-17 November 2021, (Poster presentation)

Ermis Proestakis, H.F. Christensen, Leonardo T.P. Meireles, A. Shamsolhodaei, "Shear wave velocity: using rock physics to reduce uncertainty", DHRTC Technology Conference 2021: Oil and Gas R&D towards 2050 - supporting the energy transition, Kolding, Denmark, 16-17 November 2021, (Poster presentation)

Einar M. Storebø, Morten L. Hjuler, Leonardo T.P. Meireles, Ida L. Fabricius, "Effect of Pyrite in water saturation evaluation of clay rich carbonate reservoirs", DHRTC Technology Conference 2021: Oil and Gas R&D towards 2050 - supporting the energy transition, Kolding, Denmark, 16-17 November 2021, (Poster presentation)

A. Mirazimi, D. Olsen, Erling Stenby, Wei Yan, "Simulation of Lab-Scale Gas Injection Experiments for a Lower Cretaceous Reservoir", DHRTC Technology Conference 2021: Oil and Gas R&D towards 2050 - supporting the energy transition, Kolding, Denmark, 16-17 November 2021, (Poster presentation)

Prinu Narayanan, Yiquin Liu, Teresa Regueira, Erling H. Stenby, Wei Yan "Reservoir Fluid Characterization on the Recombined Sample From Lower Cretacious Reservoir in Valdemar Field", DHRTC Technology Conference 2021: Oil and Gas R&D towards 2050 - supporting the energy transition, Kolding, Denmark, 16-17 November 2021, (Poster presentation)

Isaac L. Appelquist, Jakob. B. Roar, Benaiah. Anabaraonye, "Basics of scaling formation", DHRTC Technology Conference 2021: Oil and Gas R&D towards 2050 - supporting the energy transition, Kolding, Denmark, 16-17 November 2021, (Poster presentation)

Isacc L. Appelquist, Randi Neerup, Jakob. B. Roar, Lucas F. F. Corrêa, Jianshio Hao, Susana. Almeida, Meng Shi, Benaiah. Anabaraonye, "Scale formation studies: A multi-disciplinary approach", DHRTC Technology Conference 2021: Oil and Gas R&D towards 2050 - supporting the energy transition, Kolding, Denmark, 16-17 November 2021, (Poster presentation)

Lucas F. F. Corrêa, Randi Neerup, Meng Shi, Jiasheng Hao, Susana R. M. Almeida, Kaj Thomsen, Philip L. Fosbøl, "Determination of Thermodynamic Properties in Complex Scale Systems: Experimental and modelling efforts to improve estimation of scale solubility in brines", DHRTC Technology Conference 2021: Oil and Gas R&D towards 2050 - supporting the energy transition, Kolding, Denmark, 16-17 November 2021 (Poster presentation)

Sindhu Vudayagiri, Johannes Liljenhjerte, Jens Vinge Nygaard, Anne Ladegaard Skov, Nicolas Von Solms, "Extended Reach Intervention with Stabilizing Supports", DHRTC Technology Conference 2021: Oil and Gas R&D towards 2050 - supporting the energy transition, Kolding, Denmark 16-17 November 2021 (Poster presentation)

2021 IEA EOR TCP Virtual Symposium, Adelaide, Australia, 30 November, 2021

Yibo Yang, Teresa Regueira, Alexander Shapiro, Erling H. Stenby, Wei Yan, "Gas diffusion coefficients in oil at high pressures", 2021 IEA EOR TCP Virtual Symposium, Adelaide, Australia, 30 November, 2021 (Oral presentation)

CERE Publications

Published or submitted in 2021

CERE 1949
"Water weakening of soft and stiff outcrop chalk induced by electrical double layer disjoining pressure"
Leonardo T.P. Meireles, Einar M. Storebø, Michael J. Welch, and Ida L. Fabricius
(International Journal of Rock Mechanics & Mining Sciences, 141 (2021) 104700)

CERE 1958
"Effect of Temperature on Stiffness of Sandstones from the Deep North Sea Basin"
Tobias Orlander, Katrine Alling Andreassen, Ida Lykke Fabricius
(Rock Mechanics and Rock Engineering, 54 (2021) 255-288)

CERE 2014
"A model for relative permeabilities under gas liberation or condensate precipitation in porous medium"
Wael Al-Masri, and Alexander Shapiro
(Transport in Porous Media, 136 (2021) 43-63)

CERE 2016
"Good reporting practice for thermophysical and thermochemical property measurements (IUPAC Technical Raport)
Ala Bazyleva, Jens Abildskov, Andrzej Anderko, Olivier Baudouin, Yury Chernyak, Jean-Charles de Hemptinne, Vladimir Diky, Ralf Dohrn, J. Richard Elliott, Johan Jacquemin, Jean-Noel Jaubert, Kevin G. Joback, Ursula R. Kattner, Georgios M. Kontogeorgis, Herbert Loria, Paul M. Mathias, John P. O´Connell, Wolfram Schröer, G. Jeffrey Smith, Ana Soto, Shu Wang, and Ronald D. Weir
(Pure and Applied Chemistry, 93(2) (2021) 252-272)

CERE 2018
"Vibrational spectra and conformations for chiral opioids in changing solvents"
Michael Bache, Karin Stibius, Rolf W. Berg, Nikolaj S. Blom, and Henrik Georg Bohr
(Applied Spectroscopy Reviews, 56(3) (2021) 242-254)

CERE 2019
"Estimating Hansen solubility parameters of organic pigments by group contribution methods"
Markus Enekvist, Xiaodong Liang, Xiangping Zhang, Kim Dam-Johansen, and Georgios M. Kontogeorgis
(Chinese Journal of Chemical Engineering, 31 (2021) 186-197)

CERE 2022
"State function-based flash specifications for open systems in the absence or presence of chemical reactions"
Fernando de Azevedo Medeiros, Erling H. Stenby, and Wei Yan
(AIChE Journal, 67 (2021) 17050)

CERE 2023
"Density modeling of high-pressure mixtures using cubic and non-cubic EoS and an excess volume method"
Wei Yan, Teresa Regueira, Yiqun Liu, and Erling H. Stenby
(Fluid Phase Equilibria, 532 (2021) 112884)

CERE 2029
"Costa Tsonopoulos - his legacy and some personal reflections on cubic equations of state and beyond"
Ioannis Tsivintzelis, Eirini Karakatsani, and Georgios M. Kontogeorgis
(Fluid Phase Equilibria, 533 (2021) 112895-)

CERE 2037
"Phase envelope calculations of synthetic gas systems with a cross-over equation of state"
Andre P. C. M. Vinhal, Wei Yan, and Georgios M. Kontogeorgis
(The Journal of Supercritical Fluids, 173 (2021) 105222)

CERE 2040
"A model for relative permeabilities under gas liberation or condensate precipitation in porous medium"
Wael Al-Masri, and Alexander Shapiro
(Transport in Porous Media 136(1), (2021) 43-63)

CERE 2041
"An open-access database of the thermophysical properties of nanouids"
Maria E. Mondejar, Maria Regidor, Joerg Krafczyk, Christian Ihmels, Bastian Schmid, Georgios M. Kontogeorgis, and Fredrik Haglind
(Journal of Molecular Liquids, 333 (2021) 115140-)

CERE 2042
"Industrial requirements for thermodynamic and transport properties: 2020"
Georgios M. Kontogeorgis, Ralf Dohrn, Ioannis G. Economou, Jean-Charles de Hemptinne, Antoon ten Kate, Susanna Kuitunen, Miranda Mooijer, Ljudmila Fele Želnik, and Velisa Vesovic
(Ind. Eng. Chem. Res., 60 (2021) 4987-5013)

CERE 2043
"Effects of resonant electromagnet fields on bio-film formation in pseudomonas aeruginosa"
Janus A. J. Haagesen, Michael Bache, Livio Giuliani, and Nikolaj Blom
(Applied Sciences, 11(16) (2021) 7760)

CERE 2046
"Water-flooding and consolidation of reservoir chalk - effect on porosity and Biot's coefficient"
T.B. Gram, F.P. Ditlevsen, K. Mosegaard, and I.L. Fabricius
(Geophysical Prospecting, 69 (2021) 495-513)

CERE 2047
"Experimental determination of relative permeabilities and critical gas saturations under solution-gas drive"
Wael Al-Masri, Alexander Shapiro
(Journal of Petroleum Science and Engineering 202 (2021) 108509)

CERE 2048
"A new approach to thermal segregation in petroleum reservoirs: Algorithm and case studies"
Hadise Baghooee, François Montel, Guillaume Galliero, Wei Yan Alexander Shapiro
(Journal of Petroleum Science and Engineering 201 (2021) 108367)

CERE 2049
"Continuous upscaling and averaging"
Alexander A. Shapiro
(Chemical Engineering Science 234 (2021) 116454)

CERE 2050
"Solid-liquid equilibria of a 30 wt % aqueous monoethanolamine solution containing urea and monoethylene glycol"
Randi Neerup, Sebastian Villadsen, Kaj Thomsen, Philip Fosbøl
(J. Chem. Eng. Data, 66 (2021), 222-233)

CERE 2051
Viscosity of binary refrigerant mixtures of R32 + R1234yf and R32 + R1243zf
Xiaoxian Yang, Hangtao Liu, Shi Hai Chen, Dongchan Kim, Fufang Yang, Arash Arami-Niya, Yuanyuan Duan
(International Journal of Refrigeration,128 (2021) 197-205)

CERE 2053
"Numerical forward modeling of the overpressure build-up in the Cenozoic section of the Central Graben in the North Sea"
Ivanka Orozova-Bekkevold, and Thomas G. Petersen,
(Journal of Petroleum Exploration and Production, 11 (2021) 1621-1642)

CERE 2054
"Chemically modified hydrate swapping and hydrate stability during multistage CO2-N2 injection schemes"
Jyoti Shanker Pandey, Saad Khan, Adam Paul Karcz & Nicolas von Solms
(Fuel, 299 (2021) 120711)

CERE 2055
"Direct visualization of CH_4/CO_2 hydrate phase transitions in sandstone pores"
Jyoti Shanker Pandey, Ørjan Strand, Nicolas von Solms, Geir Ersland, and Stian Almenningen
(Crystal Growth and Design, 21(5) (2021) 2793-2806)

CERE 2056
"Chemically influenced self-preservation kinetics of CH_4 hydrates below the sub-zero temperature"
Jyoti Shanker Pandey, Saad Khan, and Nicolas von Solms
(Energies, 14 (2021) 6765)

CERE 2057
"Modeling the thermal conductivity of hydrofluorocarbons, hydrofluoroolefins and their binary mixtures using residual entropy scaling and cubic-plus-association equation of state"
Hangtao Liu, Fufang Yang, Xiaoxian Yang, Zhen Yang, Yuanyuan Duan
(Journal of Molecular Liquids, 330 (2021) 115612)

CERE 2058
"Analysis of the thermodynamic performance limits of the organic Rankine cycle in low and medium temperature heat source applications"
Fubin Yang, Fufang Yang, Jian Li, ShuoZhuo Hu, Zhen Yang, Yuanyuan Duan
(Science China Technological Sciences, 64(8) (2021) 1624-1640)

CERE 2059
"Improving the Anaerobic Digestion of Swine Manure through an Optimized Ammonia Treatment: Process Performance, Digestate and Techno-Economic Aspects"
A. Lymperatou, N.B. Rasmussen, H.N. Gavala, I.V. Skiadas
(Energies, 14 (2021) 787)

CERE 2060
"Commodity chemical production from 3rd generation biomass: A techno-economic assessment of lactic acid production"
Elena Tomas Grasa, O. Ögmundarson, N. H. Gavala, and S. Sukumara
(Biofuels Bioproducts & Biorefining, 15 (2021) 257-281)

CERE 2062
"Gas biological conversions: the potential of Syngas and Carbon Dioxide as production platforms"
H. N. Gavala, A. Grimalt-Alemany, K. Asimakopoulos, and I. V. Skiadas
(Waste and Biomass Valorization, 12 (2021) 5303-5328)

CERE 2101
"Application of quantum chemistry insights to the prediction of Phase Equilibria in associating systems"
John Towne, Xiaodong Liang, and Georgios M. Kontogeorgis
(Ind. Eng. Chem., 60 (2021) 5992-6005)

CERE 2102
"Towards a predictive Cubic Plus Association equation of state"
Pedro Velho, Xiaodong Liang, Eugénia A. Macedo, Elena Gómez and Georgios M. Kontogeorgis
(Fluid Phase Equilibria, 540 (2021) 113045)

CERE 2103
"Pore-scale visualization of CH_4 gas hydrate dissociation under permafrost conditions"
Jyoti Shanker Pandey, Stian Almenningen, Nicolas von Solms, and Geir Ersland
(Energy Fuels, 35 (2021) 1178-1196)

CERE 2104
"Solid-liquid equilibria of 30 wt% aqueous monoethanolamine (MEA) solution containing urea and monoethylene glycol (MEG)"
Randi Neerup, Dennis S. Kloth, Susana Almeida, Jens K. Jørsboe, Sebastian N. B. Villadsen, Philip L. Fosbøl
(Journal of Chemical and Engineering Data, 66(3) (2021) 1231-1237)

CERE 2105
"Ionic liquid-based in situ product removal design exemplified for an acetone-butanol-ethanol fermentation"
Yuqiu Chen, Nipun Garg, Hao Luo, Georgios M. Kontogeorgis, John M. Woodley
(Biotechnol Progress, 37 (2021) 3183)

CERE 2106
"Water-hydrocarbon phase equilibria with SAFT-VR Mie equation of state"
Nefeli Novak, Georgios M. Kontogeorgis, Marcelo Castier, Ioannis Economou
(Ind. Eng. Chem. Res., 60 (2021) 5278-5299)

CERE 2107
"Quantification of dipolar contribution and modeling of green polar fluids with the polar Cubic-Plus-Association equation of state"
Chenyang Zhu, Maogang He, Xiangyang Liu, Georgios M. Kontogeorgis and Xiaodong Liang
(ACS Sustainable Chem. Eng., 9 (2021) 7602-7619)

CERE 2108
"Solid-liquid equilibrium and binodal curves for aqueous solutions of NH_3, NH_4HCO_3, MDEA, and K_2CO_3
Lucas Farias Falcchi Corrêa, Kaj Thomsen, and Philip Loldrup Fosbøl
(J. Chem. Eng. Data, 66 (2021) 3038-3046)

CERE 2109
"Modelling study on phase equilibria behavior of ionic liquid-based aqueous biphasic systems"
Yuqiu Chen, Xiaodong Liang, John M.Woodley, Georgios M. Kontogeorgis
Chemical Engineering Science, 247 (2022) 116904)

CERE 2110
"Optimal design of an ionic liquid (IL)-based aromatic extractive distillation process involving energy and economic evaluation"
Yang Lei, Yuhang Zhou, Zhiqiang Wei, Yuqiu Chen, Fen Guo, and Wei Yan
(Ind. Eng. Chem. Res. 2021, 60, 3605−3616)

CERE 2111
"A simple model for estimating hydrogen sulfide solubility in aqueous alkanolamines in the high pressure-high gas loading region"
Humbul Suleman, Kaj Thomsen, Philip Loldrup Fosbøl, Abdulhalim Shah Maulud & Rizwan Nasir
(Journal of Sulfur Chemistry, 42(4) (2021) 410-425)

CERE 2112
"Identifying the key system parameters of the organic Rankine cycle using the principal component analysis based on an experimental database"
Dong Yan, Fubin Yang, Fufang Yang, Hongguang Zhang, Zhiyi Guo, Jian Li, Yuting Wu
(Energy Conversion and Management, 240 (2021) 114252-)

CERE 2113
"Probabilistic Approach for Risk Assessment of CO_2 Storage"
Ivanka Orozova-Bekkevold
(Internal Report - A project under DHRTC's Sprint programme 2020)

CERE 2114
"Separation of NH_3/CO_2 from melamine tail gas with ionic liquid: Process evaluation and thermodynamic properties modelling"
Xinyan Liua, Yuqiu Chen, Shaojuan Zeng, Xiangping Zhang, Xiaodong Liang, Rafiqul Gani, Georgios M. Kontogeorgis
(Separation and Purification Technology, 274 (2021) 119007)

CERE 2115
"In vivo uptake of antisense oligonucleotide drugs predicted by ab inito quantum mechanical calculations"
Henrik Frydenlund Hansen, Nanna Albaek, Bo Rode Hansen, Irene Shim, Henrik Bohr, and Troels Koch
(Nature, 11 (2021) 6321)

CERE 2116
"Benchmarking of separation methods for bioethanol (<5 wt%) recovery"
Mauro Torli, Luydmila Geer, Georgios M. Kontogeorgis, Philip Fosbøl
(Ind. Eng. Chem. Res., 60 (2021) 5924-5944)

CERE 2118
"Carbon Sequestration Through Syngas Biomethanation Coupled with H_2 Supply for a Clean Production of Natural Gas Grade Biomethane"
K. Asimakopoulos, A. Grimalt-Alemany, C. Lundholm-Hoeffner, H.N. Gavala,
I.V. Skiadas
(Waste and Biomass Valorization, 12(11) (2021) 6005-6019)

CERE 2119
"Cyclic depressurization-driven enhanced CH_4 recovery after CH_4-CO_2 hydrate swapping"
Jyoti Shanker Pandey, Charilaos Karantonidis, Qian Ouyang, and Nicolas von Solms
(Energy Fuels, 35 (2021) 9521-9537)

CERE 2121
"Scale up study of a thermophilic trickle bed reactor performing syngas biomethanation"
Konstantinos Asimakopoulos, Martin Kaufmann-Elfang, Christoffer Lundholm-Høffner, Niels B.K. Rasmussen, Antonio Grimalt-Alemany, Hariklia N. Gavala, Ioannis V. Skiadas
(Applied Energy, 290 (2021) 116771)

CERE 2122
"Solubility and freezing points of disodium terephthalate in water - ethylene glycol mixtures"
Amirali Rezazadeh, Kaj Thomsen, Hariklia N. Gavala, Ioannis V. Skiadas, Philip Fosbøl
(J. Chem. Eng. Data, 66 (2021) 2143-2152)

CERE 2123
"Thermodynamic analysis of working fluids: What is the highest performance of the sub- and trans-critical organic Rankine cycle?"
Yang Fufang, Yang Fubin, Liu Qiang, Chu Qingfu, Yang Zhen, Duan Yuanyuan
(Energy, 241 (2022) 122512)

CERE 2125
"Industrial requirements for thermodynamic and transport properties"
Georgios M. Kontogeorgis, Ralf Dohrn, Ioannis G. Economou, Jean-Charles de Hemptinne, Antoon ten Kate, Susanna Kuitunen, Miranda Mooijer, Ljudmila Fele Žilnik, and Velisa Vesovic
(Ind. Eng. Chem. Res., 60 (2021) 4987−5013)

CERE 2126
"Investigation of the performance of e-CPA for a wide range of properties for aqueous NaCl solutions"
Martin Due Olsen, Georgios M. Kontogeorgis, Xiaodong Liang, Nicolas von Solms
(Fluid Phase Equilibria, 548 (2021) 113167)

CERE 2127
"Scale attachment and detachment: The role of hydrodynamics and surface morphology"
Isaac A. Løge, Jakob R. Bentzon, Christopher G. Klingaa, Jens H. Walther, Benaiah U. Anabaraonye, Philip L. Fosbøl
(Chemical Engineering Journal, 430 (2022) 132583)

CERE 2128
"RAND-based geochemical equilibrium algorithms with applications to underground geological storage of CO_2"
Fernando de Azevedo Medeiros, Erling Halfdan Stenby, Wei Yan
(Advances in Water Resources 152 (2021) 103918)

CERE 2129
"Saturation point and phase envelope calculation for reactive systems based on the
RAND formulation"
Fernando de Azevedo Medeiros, Erling Halfdan Stenby, Wei Yan
(Chemical Engineering Science, 247 (2022) 116911)

CERE 2130
"Computer-Aided design of formulated products"
Georgios M. Kontogeorgis, Spardha Jhamb, Xiaodong Liang, Kim Dam-Johansen
(in Current Opinion in Colloid and Interface Science, 57 (2022) 101536)

CERE 2131
"ORP control for boosting ethanol productivity in gas fermentation systems and dynamics of redox cofactor NADH/NAD+ under oxidative stress"
Antonio Grimalt-Alemany, Christina Etler, Konstantinos Asimakopoulos, Ioannis V. Skiadas, Hariklia N. Gavala
(Journal of Co_2 Utilization, 50 (2021) 101589)

CERE 2132
"Computer-aided design and solvent selection for organic paint and coating formulations"
Markus Enekvist, Xiaodong Liang, Xiangping Zhang, Kim Dam-Johansen, Georgios M. Kontogeorgis
(Progress in Organic Coatings, 162 (2021) 106568)

CERE 2133
"Thermal conductivity measurements and correlations of pure R1243zf and binary mixtures of R32 + R1243zf and R32 + R1243yf"
Dongchan Kim, Hangtao Liu, Xiaoxian Yang, Fufang Yang, Jackson Morfitt, Arash Arami-Niya, Mincheol Ryu, Yuanyuan Duan, Eric F. May
(International Journal of Refrigeration, 131 (2021) 990-999)

CERE 2134
"Importance of the Relative Static Permittivity in electrolyte SAFT-VR Mie Equations of
State"
Pierre J. Walker, Xiaodong Liang, Georgios M. Kontogeorgis
(Fluid Phase Equilibria, 551 (2022) 113256)

CERE 2135
"The role of surfactants in gas hydrate management"
Jyoti Shanker Pandey, Adam Paul Karcz, and Nicolas von Solms
(Chapter in book "Surfactants in upstream E&P, Edited by Muhammad Shahzad Kamal & Syed M.

Shakil Hussain, Springer Nature Switzerland AG, (2021) 403-440)

CERE 2136
"New insights into the dissociation of mixed CH_4/CO_2 hydrates for CH_4 production and CO_2 storage"
Jyoti Shanker Pandey, Qian Ouyang, and Nicolas von Solms
(Chemical Engineering Journal, 427 (2022) 131915)

CERE 2137
"Solid-Liquid Equilibrium and Binodal Curves for Aqueous Solutions of NH_3, NH_4HCO_3, MDEA, and K_2CO_3"
Lucas Farias Falcchi Corrêa, Kaj Thomsen, and Philip Loldrup Fosbøl
(Journal of Chemical and Engineering Data, 66 (2021) 3038-3046)

CERE 2138
"On the 1D problems of carbon dioxide flow in the aquifer"
Alexander A. Shapiro
(Submitted for publication)

CERE 2139
"Vertical and lateral equilibrium in a Lower Cretaceous reservoir"
Hadise Baghooee,François Montel,Alexander Shapiro
(Journal of Petroleum Science and Engineering, 212 (2022) 110293)

CERE 2140
"Prediction of Phase Equilibria of Li-Na-K-Mg-Cl-SO_4-H_2O System at Multiple Temperatures"
Cui Rui-zhi, Nie Guo-liang, Li Jun, Kaj Thomsen, Li Wu
(Journal of Salt Lake Research, 29 (2021)1-19)

CERE 2141
"An analysis of the parameters in the Debye-Hückel theory"
Li Sun, Qun Lei, Baoliang Peng, Georgios M. Kontogeorgis, and Xiaodong Liang
(Fluid Phase Equilibria, 556 (2022) 113398)

CERE 2142
"Mass transfer between fluid particles and liquid media: A review of the available correlations with a focus on bubbles"
Mauro Torli, Miriam Lofaro, Georgios M. Kontogeorgis, and Philip Fosbøl
(Submitted for publication)

CERE 2143
"Novel visualization insights during CO2 injection into CH4 hydrate saturated porous media using a high pressure micromodel"
Jyoti Shanker Pandey, Ørjan Strand, Nicolas von Solms, Geir Ersland, and Stian Almenningen
(Submitted for publication)

CERE 2144
"A review of electrolyte equations of state with emphasis on those based on cubic and cubic-plus-association (CPA) models"
Georgios M. Kontogeorgis, Anders Schlaikjer, Martin Due Olsen, Bjørn Maribo-Mogensen, Kaj Thomsen, Nicolas von Solms, and Xiaodong Liang
(International Journal of Thermophysics 43(4) (2022) 54)

CERE 2145
"Comparison of models for the prediction of the electrical conductivity of electrolyte solutions"
Saman Naseri Boroujeni, Xiaodong Liang, Bjørn Maribo-Mogensen, and Georgios M. Kontogeorgis
(Industrial and Engineering Chemistry Research, 61(8) (2022) 3168-3185)

CERE 2146
"Conclusions from Round Table Discussion Electrolyte during IUT of ESAT 2021 Electrolyte thermodynamics challenges – from industrial needs to academic research"
Georgios M. Kontogeorgis, Antoon ten Kate, Martha Hajiw-Riberaud, and Jean-Charles de Hemptinne
(Fluid Phase Equilibria, 556 (2022) 113399)

CERE 2147
"Water structure, properties and some applications – A review"
Georgios M. Kontogeorgis, Andrew Holster, Nomiki Kottaki, Evangelos Tsochantaris, Frederik Topsøe, Jesper Poulsen, Michael Bache, Xiaodong Liang, Nikolaj Sorgenfrei Blom, and Johan Kronholm
(Submitted for publication)

CERE 2148
"Role of calorimetry in clathrate hydrate research"
Jyoti Shanker Pandey, Asheesh Kumar, and Nicolas von Solms
(Submitted for publication)

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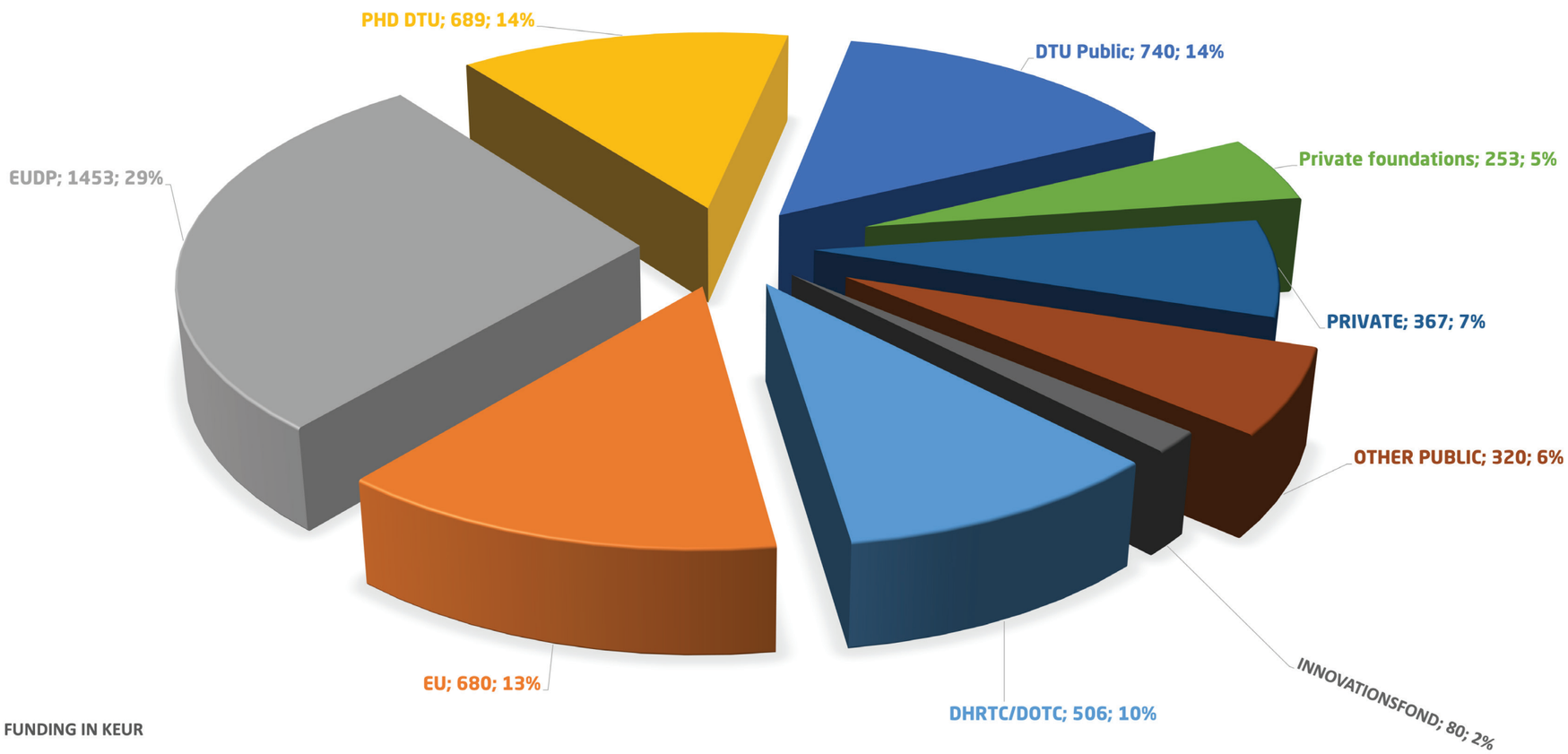

2021 FUNDING IN KEUR