# CERE Annual Report 2022

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Cover:
"The picture shows liquid samples taken from CERE's carbon capture pilot plant over three weeks. The liquids used for carbon capture are commonly referred to as "solvents". The pictured solvent is a mixture of N-methyldiethanolamine (MDEA), piperazine (PZ) and water. This solvent was used to capture $CO_2$ from biogas at Hashøj Biogas A/S, to yield high purity methane. To continue operation of the carbon capture plant, the solvent has to be regenerated in a stripper column. The stripper column is operated at around 120 °C to release $CO_2$ from the solvent, but these high temperatures also cause the solvent to degrade over time. The degradation of the solvent can be seen visually as the solvent turns yellow-brown due to degradation products. This change in color can be observed in the picture going from left (at the start) to the right (after three weeks). "



# CONTENT

# A breakthrough year for carbon capture

Some twenty years ago, researchers in CERE had an idea for a simple set-up suitable for testing carbon capture. Political interest in Denmark on the subject was close to non-existent, but since the equipment was cheap and a few students volunteered to operate it, we decided to go ahead. Admittedly, the expectations were not high. Fast forward to today: CCUS (carbon capture utilization and storage) is widely recognized as a necessary transitional step in-between the fossil present and the renewable future, both nationally in Denmark and on a European level. And at CERE, we have a range of projects covering capture, transport, utilization, and storage of $CO_2$.

Demonstrating a 30 % reduction in energy consumption, which is the largest operational cost for carbon capture, and with a leading role in the ambitious Danish CCUS scheme, 2022 truly was a breakthrough year for CERE within carbon capture. Consequently, the annual report reflects this through a section dedicated to coverage of our contributions to solving one of the most important global societal challenges of our time.

A similar societal challenge was addressed in July, as the WasteEng2022 conference took place at DTU. The bi-annual WasteEng series has evolved into the world's leading conference on Waste and Biomass Valorization. CERE was proud to co-host, yet another confirmation of our commitment to sustainable chemical engineering solutions.

**Drones and computer science aid green transition**

Obviously, it is not possible to present all the successes from the many projects in CERE in a single report. Still, remarkable progress in the field of using drones for magnetometer surveys could not be overlooked. The novel drone systems can identify unexploded ordnance (UXO) and contribute to the search for valuable minerals. Notably, both these applications are related to green transition: UXO is a major safety hazard and economic burden to construction of offshore windmill farms, while minerals are necessary to manufacturing of batteries for electric vehicles, photovoltaic cells etc.

In an abstract sense, the use of drones in these somewhat unexpected applications speaks to the nature of research: scientific excellence often tends to prove valuable in fields that are seemingly far from the original scope. A similar example can be found for the research in CERE on Model Predictive Control (MPC). Motivated by the complex challenges involved in producing optimally across hydrocarbon offshore fields, we got involved in MPC a decade ago. Now, it has transpired that MPC is equally relevant to a range of other industrial contexts, one of them being CCUS. Processes where $CO_2$ is either stored in subsurface reservoirs, applied in Enhanced Oil Recovery, or utilized in Power-to-X or other applications depending on market conditions and the quality of the captured $CO_2$ involve extremely complex challenges which will require advanced software tools such as MPC.

**Discussion Meeting back in the physical format**

Most readers of the annual report will probably know that the CERE Discussion Meeting is where we invite members of the CERE industry Consortium and other stakeholders to meet our faculty and staff for presentations on cutting edge research and frank discussions on future topics and approaches.

As reflected in interviews with participants over the following pages, the contributions from CERE to green transition was an underlying theme.

Discussing our work with industry and other stakeholders is not only enjoyable but also essential to ensuring the continued relevance of what we do. An example highlighted in this report is the longstanding collaboration with Equinor on thermodynamic modelling for gas processing applications. Many other joint industry projects could have been chosen – and certainly will be in coming annual reports.

On a personal note, I would like to emphasize how pleased I was to see the Discussion Meeting back in the physical format. Regardless of the advantages that online conferencing has brought us, it was a pleasure to be able to meet all of you in person again!

Nicolas von Solms
CERE Chairman
Professor, DTU Chemical Engineering

# Industry Consortium

## The Consortium – our Strongest Asset

CERE is supported by public funding 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 23 companies are members, the number changes due to the dynamics of the industry. The member companies closely follow the activities of our center. This ensures that CERE activities are relevant in relation to the research we do. This ongoing external control of quality and inspiration assist in maintaining CERE research at the highest international level.

### We welcome Baker Hughes

Baker Hughes is an international industrial service company and one of the world's largest oil field service companies. The company provides the oil and gas industry with products and services for oil drilling, formation evaluation, completion, production and reservoir consulting.
Baker Hughes has a strong emphasis on carbon capture and storage (CCS). Collaborations with CERE will primarily be within CCS. Particularly, Baker Hughes is interested in CERE's longstanding expertise in extended UNIQUAC for thermodynamic modelling and speciation in carbon capture processes. CERE's experience with this model and with electrolytes in general is enhanced and underpinned by an extensive electrolyte database, compiled over many years, originally by Associate Professor, now Emeritus, Kaj  Thomsen. Work on CCS and electrolyte thermodynamics remain highly active fields for several faculty in CERE.

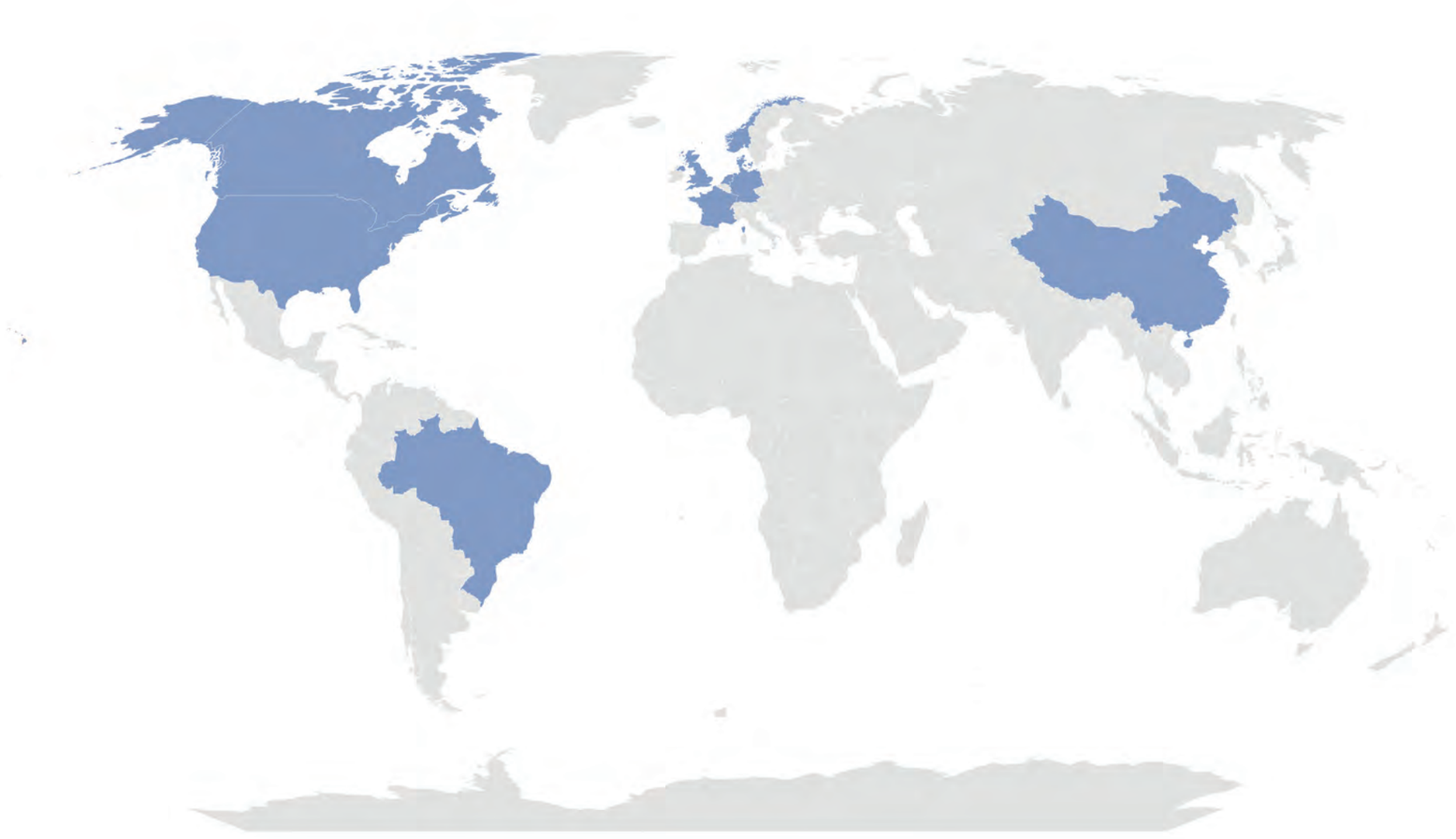
### We welcome ESSS

Headquartered in Florianopolis, Brazil, Engineering Simulation and Scientific Software (ESSS) is an international company offering advanced computer-aided engineering (CAE) tools in fluid dynamics, structural analysis, electromagnetism, and multiphysics, including customized software.
ESSS offers simulation solutions for more than 700 clients in sectors such as aerospace, mining, and automotive. Further, ESSS is an Ansys Elite Channel Partner and the official Ansys software provider for Latin America, Portugal, and Spain.
Extensive collaboration with academia is a part of the company strategy. Currently, more than 3,000 academics use ESSS simulation software for phenomena related to fluid characterization, production, and flow assurance, from concept and design to testing and validation.

### We welcome Schlumberger back

Schlumberger is the world's largest service provider for the energy sector and a longstanding member of the CERE industry Consortium. Due to a general downturn for the industry, Schlumberger paused its membership but is now back with us. We look forward to resuming the collaboration.

# CERE Consortium



Aveva - UK

Baker Hughes - USA

BP - UK

Calsep -DK

Chevron - USA

Sinopec - China

Dan-Unity - DK

DSM - Netherlands

Equinor - Norway

ESSS NA - Brazil

IFPEN  - France

KBC - UK

Linde - Germany

Schlumberger -  Canada

Shell - Netherlands

Total Energies - France

Union Engineering / Pentair - DK

Wintershall – Germany

# DISCUSSION MEETING

# Discussions on green transition


*CERE Discussion Meeting 2022*

**After two years of pandemic, CERE could again welcome stakeholders to a physical version of the annual Discussion Meeting with green transition in the energy resources sector as backdrop.**

*Dr. Kurt Schmidt, Schlumberger*

Any CERE Discussion meeting will have an element of reunion – saying hello again to former colleagues, students, and professors. To Dr. Kurt Schmidt of Schlumberger this was especially true for the 2022 version:

"Well, with COVID and all it is nice to be able see everybody again, face-to-face, over a cup of coffee. Furthermore, due to a general downturn for the industry we paused our membership of the CERE industry Consortium. Now we are back – we still see  value in our engagement."

Schlumberger is the world's largest service provider for the energy sector.

"The membership in general and this conference in particular is an opportunity for us to provide input on the future research projects within thermodynamics and transport properties both fundamental and applied."

While the core business of Schlumberger remains traditional hydrocarbon field services, several other areas have become of interest in recent years.

"Hydrogen, CCUS (carbon capture, utilization, and storage), energy transition – just to name a few. I am happy to see that these topics are all prominently addressed at the conference. That wasn't so much the case when I was here the last time, four years ago. It is nice to see CERE addressing these fields with confidence – showing that "we know how to do this". It is apparent that the gauntlet has been picked up," Kurt Schmidt comments.

## Broadening the scope

IFP Energies Nouvelles (IFPEN) is a long-standing member of the CERE industry consortium. IFPEN is a private group created by the French state and relying both on public and private funding. Most of the private income originates from sales of subsidiaries, based on license agreements for patented inventions.

*Dr. Jean-Charles de Hemptinne, IFPEN*

"Coming originally from oil and gas exploration and use, we - just like many energy corporations, and like CERE - are broadening our scope to encompass for example new energy sources (bioresources, wind or geothermal energy), carbon capture and storage technologies, energy storage technologies (hydrogen economy, gas storage in salt caverns or batteries) and increasingly the circular economy (recycling of polymers or metals). These applications require processes in sometimes extreme conditions, and therefore an advanced understanding of thermodynamic modelling tools," says Dr. Jean-Charles de Hemptinne, IFPEN.

The current transformation is in accordance with societal demands, Dr. de Hemptinne continues:

"We are quite successful I would say, when it comes to finding ways to use our skills within new fields. The main challenge lies in the time horizons. In research, one needs to be able to plan many years ahead. for the minimum time is three years since this is the duration of a PhD project. However, this is not always possible. Take biofuels as an example. In the years after 2000, the interest in biofuels was high but somehow political attention evaporated when the competition with the food markets became too strong. Something similar happened to carbon capture – which now has reentered the scene to make a strong comeback. These fluctuations are challenging since it typically takes some years to get from research to a level which can be applied in industry."

## A business card in Arabic

Possibly as the only participant at the CERE Discussion Meeting 2022, Ioannis Economou can present a business card in Arabic. He is Professor of Chemical

*Professor Ioannis Economou,Texas A&M University, Qatar*

Engineering at Texas A&M University, USA, but working out of the Qatar campus in Doha.

"To my mind, the most important thing is that we as thermodynamics researchers continue to work closely with industry. Recent years have seen a trend where the industry thermodynamics groups are shrinking. For instance, several of the large international energy corporations have reduced the sizes of their groups. Instead, companies are relying more on university collaborations. This is a nice thing for us on the academic side. You might even say that this is a natural division of work. But it also increases our responsibility when it comes to assuring that our projects are relevant to the industrial practice."

Ioannis Economou has been associated with CERE for more than two decades. The connection was established in 1999 when he, then as Research Director in "Demokritos" Research Center in Greece, visited the research center IVC-SEP (that later transformed into CERE) where he did two sabbaticals


over the following years. Later, the relationship with CERE developed further, and several students from DTU have spent time in his group and vice versa.

"Like many other groups coming from petroleum research, CERE is undergoing a transition to a broader interest which includes clean energy and sustainable processes. CERE has been successful in attracting several grants from Danish funding agencies, the EU and from industry, and is today at the forefront of these transitional technological developments," says Professor Economou.

"Since Denmark is a small country, its implementation of new sustainable energy systems and industrial processes may not in itself have that much impact on a global scale. Still, by setting an example in these areas I believe the impact is actually very significant worldwide."

**Resuming conversations**

With a dual background in chemical engineering and physics, Dr. Kurt Schmidt is the Digital Lead for System Performance where he takes care of new product development projects for Process Optimization in Facility Digital Twins at Schlumberger:

"Our work is to a high degree determined by requests from clients. For instance, we are currently working on digital twins for process facilities which monitor and optimize facility operations remotely.



Optimization in these projects is subject to numerous constraints such as revenue, energy efficiencies, and emissions."

The CERE Discussion meeting 2022 provided several presentations within digital twins, control software, and carbon dioxide capture, utilization, and sequestration which align with his current role. While these applications are useful to him, another topic remains a top priority for Kurt Schmidt:

"Although the final results of the applications are interesting, my main interest is ensuring that the underlying models - the thermodynamic and transport properties fundamentals if you will – are correct and can be utilized in an appropriate architecture for the applications."

Having that preference, Dr. Schmidt has come to the right spot:

"This is much like meeting up with old friends. Okay, the students will come and go but the professors and many of my industry colleagues are familiar faces. It feels like we can resume conversations that have just been interrupted for a few years."

**The CERE Discussion Meeting 2022 was held June 6-10 at the Comwell Borupgaard conference center in Snekkersten, Denmark.**

# Drone-based search for minerals

*Senior Researcher Arne Døssing Andreasen*



# Novel drone improves the hunt for minerals

## A patented triple-sensor magnetometer system makes geological mapping by drone more accurate than traditional aerial methods.

Green transition requires minerals for the batteries of electric cars, solar cells, and wind power storage. In a world with a huge appetite for minerals, better ways to locate underground resources is in high demand. A research group led by CERE faculty member Arne Døssing Andreasen has developed a drone payload system for the purpose, already in use by mining industry.

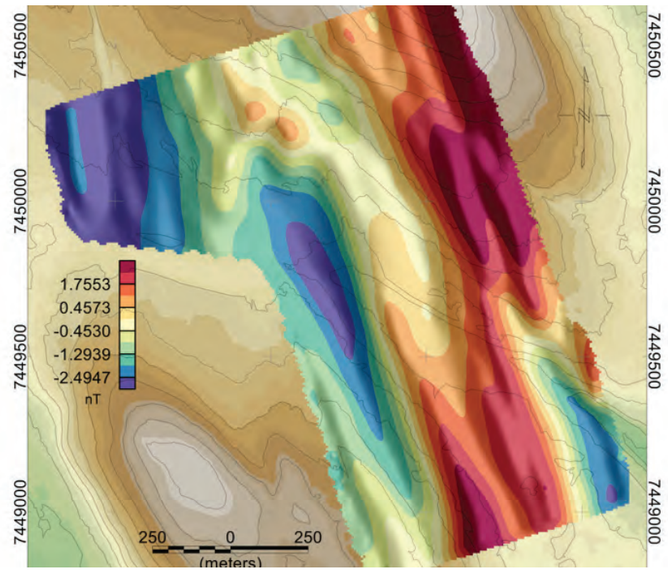
"Since both the reliability and the operational range of drones have improved significantly over recent years, it is very natural to see if they can be applied to geomagnetic surveying," says Arne Døssing Andreasen, Senior Scientist at DTU Space.

Geomagnetic surveying is by far the fastest way to obtain detailed information about the underground. Variations in the strength of the Earth's magnetic field reflect the geological structures. Thereby, mining companies can pinpoint locations that seem promising rather than drill randomly.

"Not surprisingly, drone surveying has proven to be a lot cheaper than traditional surveying by plane or helicopter. But on top of the improved economic feasibility, we have also demonstrated higher resolution and data quality," says Arne Døssing Andreasen.

### Already applied in Nickel exploration

One industry partner, Australian mining company Ofoten Minerals Ltd., has already applied data acquired by the new drone system.




*Magnetic anomaly data from on a drone magnetic gradiometry survey in relation to an iron oxide copper-gold mineralization, Nautanen (Sweden)*

"We surveyed an area in Northern Norway, where the company had older data acquired through helicopter surveying. The idea was just to compare the two types of surveying and see if the drone data had sufficient quality. It transpired that the drone data had much better resolution than the helicopter data, leading the company to revise its understanding of the geology. Accordingly, they have now changed their plans on where to drill."

The location in question is rich in Nickel which is a key mineral in production of batteries for electric vehicles.

In another project, the research group has developed a drone system for identifying unexplored ordnance (UXO) offshore (see the article on the PhD project of Mark David Wigh in the PhD Thesis section). This drone system has been the starting point for development of the new drone system for minerals exploration. Still, some features are different, Arne Døssing Andreasen explains:

"When you want to map potential mineral resources in the underground, you are typically looking at a large area. Much larger than in the case of UXO identification which is normally done for instance at a construction site for a windmill

park. So, for minerals exploration we need a drone able to fly quite far and to be quite autonomous."

weighs 25 kg of which 4.5 kg is the sensor system, which has been patented by Arne Døssing Andreasen.

"Uniquely, the three sensors measure the Earth's magnetic field in three different directions. This has not been done before at this accuracy in a drone system. Measurements in multiple directions will yield more information, and is the main reason why we have succeeded in making the drone system more accurate than helicopter surveying," says Arne Døssing Andreasen.

Further, accuracy is improved by the drone flying closer to the ground than a plane or a helicopter would. The drone sensor system developed at DTU will typically maintain a constant altitude of 30 meters above the ground, adjusting to variations in the terrain height, while the drone itself is at 10-meter higher altitude to avoid electromagnetic disturbances from the drone in the magnetic measurements.

*Picture of a heavy-lift drone (Narvik, Norway) used for towing the magnetic payload for mineral exploration purposes.*

**Adjusting to variation in terrain height**

In the current configuration, the new drone system is able to fly up to 40 minutes per flight. This equals a fly range of 25 kilometers. The drone

**Keen to survey Swedish meteor crater**

"We are keen to survey a crater which was created by the impact of a meteor. Such craters are known to often have various types of exotic minerals."

The project currently has funding for another 1.5 years, but Arne Døssing Andreasen hopes it will be possible to obtain funding for the development of drone systems for minerals exploration beyond that time horizon:

"I feel certain that the future of airborne minerals exploration belongs to drones. Currently, helicopter surveying remains the dominant method but given that you need specialized helicopters and especially trained crews this is expensive with limited capacity. Drones can be operated far more easily, cheaply, and with higher flexibility. Further, we have demonstrated a higher accuracy."

Besides Northern Norway, the drone has flown in Iceland, Northern Sweden, and in Greenland. One of several future projects relates to a site in northern Sweden, the Senior Scientist reveals:

CCUS

CARBON CAPTURE UTILIZATION AND STORAGE

*Ph.D. Student Jens Kristian Jørsboe*

*Associate Professor. Philip L. Fosbøl*

*Ph.D. Student Randi Neerup*

# Leap forward in carbon capture

**CERE researchers have demonstrated 30 % savings in the energy consumption needed for carbon capture. Thereby, costs are reduced, and economic feasibility significantly improved.**

During months of operation, a mobile test unit designed by CERE researchers has been consistently able to capture $CO_2$ with 30 % less energy consumption compared with state-of-the-art in the field. Since energy is the number one cost during operation, savings of this order improve the economic feasibility of carbon capture greatly.

"We had shown in simulations that energy savings of this order were possible. Still, being able to achieve these results in practice is highly satisfying," says Ph.D. student Jens Kristian Jørsboe, CERE.

Design of the mobile unit was coordinated by Associate Professor Philip L. Fosbøl, CERE, while industry partner Union Engineering constructed the unit.

The unit can capture 1.0 ton of $CO_2$ per day.

"Although this is pilot scale, at this level of operation, we encounter many of the problems, which are likely to occur under real carbon capture implementation," notes Jens Kristian Jørsboe.

The mobile unit is currently installed at the largest cement kiln at Aalborg Portland cement factory. Here, the unit will be tested by Aalborg Portland until October 2023, as the basis for a full-scale facility.

"This project is to develop new technology that will reduce $CO_2$ emissions and contribute to a more climate-friendly cement production in Denmark. This is a unique opportunity to test this technology at a company that plays such a large role in the climate change agenda," says Philip L. Fosbøl.

## Spare process heat can be utilized

Previously, the unit was operated at Amager Resource Center (ARC), Hashøj Biogas, and Mølleåværket.

Notably, the unit was able to achieve the same high level of efficiency at three different locations with different carbon sources. Amager Resource Center (ARC) produces heat from waste incineration, while Hashøj Biogas and Mølleåværket produce biogas from ma-

nure and wastewater.

"If we, as hoped, can achieve


*Carbon capture pilot plant*

the same high energy efficiency for flue gas from cement production, which is quite different from waste incineration and from biogas, we will be able to say with confidence that our technology is able to save energy universally for carbon capture," says Jens Kristian Jørsboe.

Looking further ahead, he imagines even larger savings in energy consumption:

"So far, the mobile unit has just been added to the already existing installations – known in chemical engineering as retrofitting. If we would be allowed to make modifications to the existing installation, we could achieve higher savings."

For example, production of heat from waste incineration at ARC and production of cement at Aalborg Portland generates process heat. This heat could become valuable in carbon capture, not least during desorption.

"This is where the savings we already have achieved become especially interesting. With 30 % savings we are not too far from the threshold, where spare process heat from an incineration plant or a cement factory or a similar installation would cover the total energy need for heating in carbon capture. This would imply the process could potentially run without external heat supply. In other words, we would have eliminated the largest operational cost," says Jens Kristian Jørsboe.

**Novel solvent mixtures**

The encouraging results cannot be attributed to one silver bullet, but rather to a combination of improvements.

Firstly, tailormade solvent mixtures are applied. The standard amines for carbon capture are MEA (mono-ethanolamine) and MDEA (methyl diethanolamine). The CERE group has instead applied a range of different mixtures consisting of two or more solvents. These include mixtures of piperazine and AMP (2-amino-2-methyl-1-propanol), known as the CESAR1 solvent, and piperazine and MDEA.

"Piperazine is very efficient when it comes to capturing $CO_2$, but since it binds the $CO_2$ relatively strongly you need to use a lot of energy later in the process when you want to desorb the $CO_2$ from the solvent. By far the largest part of the energy consumption in carbon capture is for heating to make the desorption work. Other amines such as MDEA and AMP have a weaker binding to the $CO_2$, thereby savings in energy consumption for desorption can be achieved using a combination of these solvents," explains Jens Kristian Jørsboe.

Secondly, the researchers have avoided several internal losses in the system. At certain stages, a low temperature is necessary, and cooling is applied. Cooling also generates heat, which was previously just wasted. The team has managed to redirect this heat and use in the later stages where heat is called for.

Finally, various optimizations based on old school chemical engineering principles have contributed to the overall result.

"Many of the improvements made are simple. Still, you need to show in practice that they work – and we are simply the first, or at least some of the first, to have done that," says Jens Kristian Jørsboe.

**Synergies are hard to catch in simulations**

Many things can be calculated, but until you have achieved your results in practice you cannot be sure:

"For instance, since we are doing many different improvements, it is hard to know what the overall result will be. Different modifications could be synergetic, yielding even better results or they could be counterproductive. These interdependencies are just very difficult to catch in simulations."

Another example is the effect of impurities, notes Jens Kristian Jørsboe:

"When you do carbon capture on gases from real industry processes, some impurities will always be present. You can try a simulate the effect of these impurities in lab experiments, but only real-life experiments will give the true picture."

Despite the promising results, the mobile unit cannot be seen as a plug-and-play solution. For example, the exact formulation of the solvent mixture needs to be modified for the application in question, explains Jens Kristian Jørsboe:

"Flue gas from a power plant, or from an incineration plant like ARC is rich on oxygen. Therefore, you need solvents that do not oxidize easily. Because if they do oxidize, you risk formation of various undesired by-products which might be harmful to health or environment. In contrast, carbon capture in connection with production of biogas is faced with very low oxygen contents since the microorganisms in these plants are largely anaerobic. However, the sulfur content is often high so for that purpose you need solvents that do not readily react with sulfur. At Aalborg Portland we will be faced with yet another totally different flue gas composition. Depending on the industry in question, and the size and design of the relevant installation, modifications will be needed."


*Carbon capture and PtX biogas cleaning demonstration plants at Hashøj biogas. The green tower in the back is the DTU carbon capture pilot plant that is part of the BioCO2 project, and the container with the blue banner in front is part of a Power-to-X gas cleaning project called BE Clean*

# Tackling corrosion is crucial

## With large scale carbon capture becoming a reality, the issues related to transportation of $CO_2$ grow in importance.

Once, the abbreviation was CCS for Carbon Capture and Storage. In recent years, CCUS has come to dominate, with the added U for Utilization. However, perhaps yet another letter should be added to give the full picture: T for Transport.

It is well established that the economic feasibility of carbon capture is much better when targeting high-emission sources such as power plants or large industrial facilities. These installations are rarely located near geological sites suited for storage. So, how to best transport the $CO_2$ to the storage sites has become a crucial issue for the overall feasibility of carbon capture.

"Capturing carbon and transporting it to a storage site is already technically possible. However, several questions which are important for the economy of the solutions are still unanswered," says Randi Neerup, Ph.D. student at CERE.

$CO_2$ is not just $CO_2$. The $CO_2$ stream can vary from 75.0 to 99.9 vol % and contain various impurities depending on the capture process, for example, solvent degradation products or residual material from the feedstock gas, anything from NOx to hydrogen. These impurities can cause unforeseen condensates, corrosion, hydrate formation, and changes in phase behavior during transport, injection, and storage of $CO_2$. Therefore, captured $CO_2$ must be conditioned and cleaned to be compatible with the transport, storage, and utilization infrastructure.

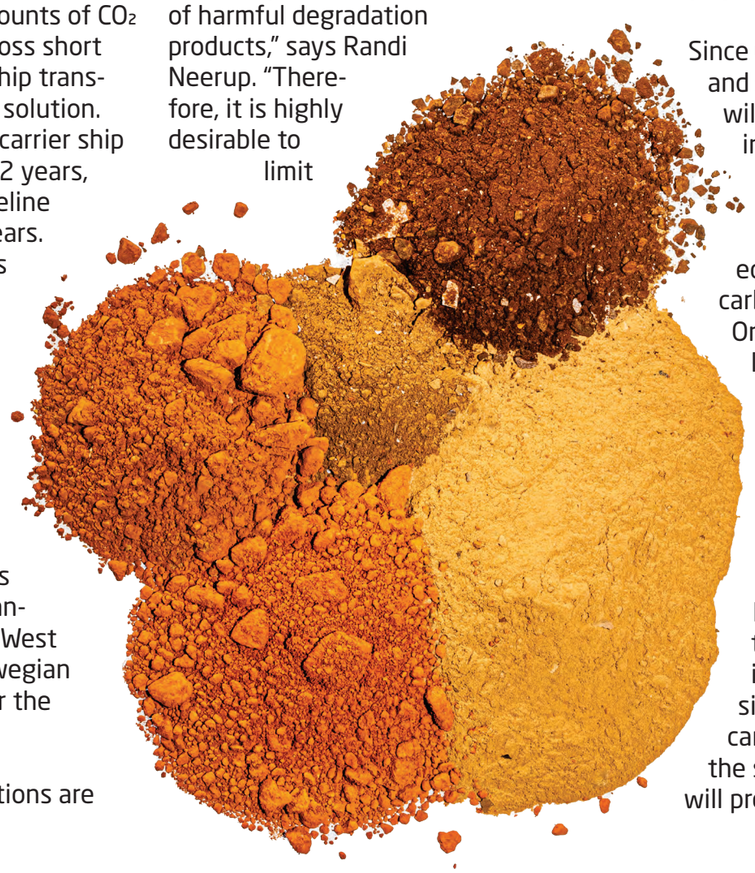
### Balancing purity against costs

$CO_2$ can be transported by pipelines, trucks, trains, or ships. Pipeline transportation offers the largest operation capacity, while shipping is most flexible. Currently, small amounts of $CO_2$ are transported across short distances leaving ship transport as the optimal solution. Constructing a $CO_2$ carrier ship can be done in 1.5-2 years, whereas a new pipeline will require 5-10 years. Shipping companies are currently working on developing $CO_2$ transport strategies, transporting to onshore facilities in Iceland or Norway or offshore, possibly for storage in depleted oil and gas reservoirs in the Danish North Sea (Nini West reservoir), the Norwegian continental shelf, or the Herald reservoir.

If the $CO_2$ specifications are not harmonized across the capture, transport, storage, and utilization infrastructure, extra conditioning will be needed. This will significantly increase the amount of energy required for handling $CO_2$ and thereby also the costs.

The phase behavior of $CO_2$ is heavily dependent on the gas purity, which is again dependent on the source of carbon capture.

"Even small amounts of impurities may lead to formation of harmful degradation products," says Randi Neerup. "Therefore, it is highly desirable to limit the amounts of impurities. But again, this is also an economic issue. And right now, it is difficult to calculate the economic feasibility since no international standard for $CO_2$ exist."



### Controlling the level of iron carbonates

In her PhD project, Randi Neerup works both on capture techniques and on prophylactic techniques relating to $CO_2$ corrosion. The latter part of the project is financed by DTU Offshore.

Since $CO_2$ is highly corrosive, and since the captured $CO_2$ will have to be transported in either steel pipes or steel tanks, addressing $CO_2$ corrosion is a key issue for the economic feasibility of carbon capture and storage. One option is limiting the level of corrosion through management of the iron carbonate level in the $CO_2$ stream.

"Having a little iron carbonate in your stream is useful, since this will help form a thin layer at the steel surface protecting against further corrosion. But if too much iron carbonate is released from the steel, the iron carbonate will precipitate inside the pipe leading to various problems. So, the idea is to keep your level of iron carbonates inside the optimal zone," Randi Neerup explains, adding that there is more to the story:
"We also need to ensure that the release of iron carbonates from the surface is not accompanied by formation of various substances which could potentially be hazardous to human health or to the environment. So, it is a complex challenge."

*PhD. Student Randi Neerup*

# A call for $CO_2$ standards

**"It is estimated that on a global scale, 5,000 Mtpa (million tons per year) of $CO_2$ will need to be permanently stored by 2050 to abate the climate crisis. In comparison, 40 Mtpa of $CO_2$ is currently stored worldwide.  Storing 5,000 Mtpa of $CO_2$ is not possible with the available storage capacity and infrastructure**

INEOS expects to operate in the Nini West reservoir in Danish North Sea. The company will use reservoirs with an existing storage capacity of 80 Mt og $CO_2$ and operate with a capacity of 8 Mtpa by 2030.  With upgrades in reservoirs and saline aquifers in the Siri area, with new platforms and pipelines, the operating capacity would be 20-50 Mtpa for 20-30 years, with a total storage capacity larger than 2 Gt of storage.

To reach 5,000 Mtpa in 2050, safe and permanent storage is a necessity. This is accomplished by well integrity management during $CO_2$ injection. Integrity depends on material properties and cementation of the wells and the chemical properties of the injected fluid. If these aspects are not properly addressed, corrosion and leakage can occur over many years of operation. Global and properly documented standards could ensure the wells would be retrofitted to accompany different levels of $CO_2$ purity or wells would be repurposed with the option of storing low- or high-grade $CO_2$ in different reservoirs. This would provide the option of balancing the cost between capture and storage sites. Furthermore, low grade $CO_2$ storage might be necessary for cases in which capture units produce $CO_2$ with high impurity levels. Impurities will therefore influence the market value of $CO_2$, as the cost of operation depends on the source and level of impurities.

$CO_2$ utilization often requires a $CO_2$ purity higher than that needed for long-term storage. For this reason, it is important that future $CO_2$ infrastructure can handle several different qualities of $CO_2$, for storage, conversion, or food. The $CO_2$ infrastructure will need to handle this aspect much more in detail, because $CO_2$ properties can have a significant impact on cost and health. It is unclear what level of impurity can be accepted for utilization, but a quality standard must be in place soon to support the growing market for alternative storage and/or conversion of $CO_2$. This information is critical knowledge for example in Ørsted, where $CO_2$ to methanol conversion is expected before 2030 on a scale of several million tons of $CO_2$ per year.

The European emission trading scheme (ETS) or any similar framework must accommodate the need for full carbon reduction independent on source where standardized $CO_2$ purities are considered. We call for additional high-purity quality standardization that is targeted to certain specific $CO_2$ utilization applications. Global coordination is needed to accommodate cross-world infrastructure opportunities. This needs to fit a trading system like ETS and will require low levels of impurities to ensure health and safety.

Building the transportation framework (for $CO_2$, ed.) imposes large up front capital investments, and without certainty about the future of CCUS from governmental bodies, the economic risk for industries will be too large. The $CO_2$ transport system is critical infrastructure and must be in place for any global $CO_2$ value chain to function. We urge the European Union and other global governments to take initiative and create a large-scale $CO_2$ transport system, to support capture and storage activities, to reduce cost (...)."



**Excerpt from the article**

**"A Call for Standards in the $CO_2$ Value Chain",**

Environmental Science & Technology, 2022,56,24,17502-17505

Corresponding author Associate Professor Philip L. Fosbøl, CERE.

Authors from industries:

- Carbfix Iceland,
- INEOS Oil & Gas Denmark,
- Amager Resource Center,
- Northern Lights,
- Horisont Energi,
- Dan-Unity $CO_2$

and several CERE researchers have contributed to the article.

# Towards full-scale carbon capture and storage

*Relocation of $CO_2$ capture plant from ARC*

**CERE researchers have been active in carbon capture through several decades regardless of fluctuations in the political interest in the field.**

Today, as many nations, including Denmark, see carbon capture as an important element in climate change mitigation, CERE is active in all the subdisciplines of the field. The involvement started a bit by chance, recalls CERE chairman, Professor Nicolas von Solms:

"At that time carbon capture didn't have much political attention, but we had an idea for a simple absorption column. We found a cheap way to get it tested through a couple of bachelor projects. Using the amine MEA (mono-ethanolamine, ed.) which was state of the art at the time to capture $CO_2$ from artificial flue gas, we could demonstrate that we had an ideal setup for testing the performance of solvents. These results were noted internationally, and we were invited to take part in an EU program called Interact."

The European funding allowed for a new so-called wetted wall column to be developed and constructed at DTU. The equipment allowed the DTU researchers to test many new techniques. For example, the performance of the enzyme carbonic hydrase in carbon capture.

"We were able to show that a small amount of carbonic hydrase with the amine solvent MDEA (methyl diethanolamine, ed.) performed as well as the baseline MEA. This was very encouraging and surprising since use of MEA had been optimized over many years."

**Arriving late for the party**

The scientific results allowed CERE to continue participation in subsequent European programs, even though Denmark did not devote much funding to carbon capture research for several years.

"Norway, USA, UK, China, and other nations became the leaders in carbon capture. I think it is fair to say that Denmark arrived a bit late for the party, but in recent years this has all changed," says Nicolas von Solms.

Coordinated by Associate Professor Philip L. Fosbøl, the CERE researchers are today active in a range of Danish carbon capture projects. These include a mobile demonstration unit at the Amager Resource Center (ARC) and at biogas plant Hashøj. Further, a large project under the national research and development program Innomission.

In the European perspective, a project demonstrating a new electricity-based carbon capture technology in Denmark, Greece, and Romania has recently been initiated. Philip L. Fosbøl coordinates the CERE participation.

Together, all these activities will contribute to the coming full-scale implementation of carbon capture both in Denmark and in a wider European context, Nicolas von Solms summarizes:

"Being chemical engineers, we are not strangers to having medium or even full-scale implementation in mind. But since we are university researchers, we also insist that we should be concerned with the basic science. Demonstrating a technique is fine, but we also want to understand what goes on. Which fundamental parameters are involved, and how are the kinetics performing? Knowing the answers to these questions is not just an academic exercise. This will be crucial for later upscaling of the processes, which is very relevant in the case of carbon capture."

**Participation in EU flagship project**

Due to their long-standing involvement and expertise, Nicolas von Solms and Philip L. Fosbøl were invited to participate in a highly ambitious European project. Eleven academic and industrial partners from six European countries are building a world-leading plant for capture of $CO_2$ at the Arcelor-Mittal steel factory in Dunkirk, France. The project is called "DMX Demonstration in Dunkirk" (or "3D" for short). DMX is a carbon capture technology patented by IFP Energies Nouvelles, overall coordinator of the 3D project.

The total budget of the 3D project is 19.3 million euro, of which the European Union's research and innovation program Horizon 2020 has supplied 14.8 million euro.

"While most of the budget is dedicated to the development of the capture plant itself, a part of the financing will be for development of transportation solutions. This is what we are responsible for," explains Nicolas von Solms.

"Since many nations share the same challenge of capture, transport, and storage of $CO_2$, it will not be rational for each project or capture facility to develop their individual logistics solution.

*Factory in Greece that is part of ConsenSUS, which deals with $co_2$ capture*

## Pros and cons for pipelines

In the 3D project, alternative sites for storage are considered in The Netherlands, UK, and Norway respectively.

"Since the Dutch location is not that far from Dunkirk, it could be feasible to establish a pipeline for the $CO_2$ transportation. But if Norway is chosen as the storage site, building a pipeline would be way too expensive. In this case, it would be necessary to liquify the $CO_2$ and establish transportation by ship," says Nicolas von Solms.

Currently, various ideas for both pipelines and seaborne transportation are in play.

Transporting $CO_2$ through a pipeline will require a very large compressor to provide the necessary pressure, but this is possible. However, in the case of $CO_2$ storage one faces an additional challenge. Initially, the pressure inside the targeted geological formation – for instance a depleted oil field in a saline aquifer offshore – will be significantly lower than the pressure of the transport stream.

"We are maybe talking about transportation at 120 bars and an internal pressure in the geological structure of 50 bars. This equals good conditions for pumping the $CO_2$ into the underground. But gradually the pressure of the reservoir will rise as $CO_2$ is injected, and it will become more costly to create the pressure difference needed to inject more $CO_2$. For how long will it be feasible to continue? We will need to look very carefully at the economy here," explains Nicolas von Solms.

## Large-scale optimization is called for

Similar issues are addressed for the transportation of liquified $CO_2$ by ship:

"Currently the standard recommendation for this type of transport is to keep your $CO_2$ under a pressure of 15 bars. However, the quantities which are transported today are much lower than in a future carbon capture scenario, and the issue has not been addressed from a large-scale optimization perspective. If we can lower the pressure to 7 bars, large amounts of steel for tanks and pipes can be saved and the overall feasibility will be significantly improved."

On top of these issues comes other technical considerations:

"Captured $CO_2$ will not be pure. Thus, you will need some level of "polishing" as it is called in the technical terminology before you either send your $CO_2$ through a pipeline or prepare it for liquification. Also, it is desirable to avoid having more than one phase in your stream. These specifications need to be worked out carefully. And again, with huge amount of $CO_2$ in the future system, small optimizations can be crucial to the overall feasibility."


*Professor Nicolas von Solms*

# Strong CERE participation in Danish Carbon capture

## A new partnership is to implement Carbon Capture Utilization and Storage (CCUS) in Denmark. CERE is involved in a range of projects.

According to the Danish government, Carbon Capture Utilization and Storage (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. Several CERE faculty members and other staff have been active in the DTU contribution to the roadmap.

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.

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.

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.

CERE is represented in several projects approved in the first round of INNO-CCUS grants. The CERE participation spans across four DTU departments (Chemistry, Chemical Engineering, Environmental and Resource Engineering and Compute).

From Environmental and Resource Engineering, Researcher Leonardo Mireiles will participate in the project "Borehole Monitoring Solutions for $CO_2$ storage wells, which run from September 2022 to September 2025. This project concerns the monitoring that can be done inside and near onshore wells. It will consider the operational needs for monitoring and describe existing technology, such as well head monitoring (pressure, temperature, flow) and technology that could be improved or adapted for the continuous monitoring of the well. The latter include the use of distributed fiber optics sensing to monitor deformation and temperature changes; and petrophysical cased hole logging technologies used to describe fluid saturation and integrity of cement and near-well rock masses. The project will seek to develop these to a proof-of-concept stage for $CO_2$ storage.

From Chemical Engineering, Associate Professor Alexander Shapiro with participate in the project "$CO_2$flow – Experimental study and modelling of $CO_2$ propagation in geological storage" The project has a duration of 12 months and is about the experimental and modeling study of the $CO_2$ injection in the aquifer, using CT scanning.

Also in DTU Chemical Engineering, the project CORT ($CO_2$ capture demonstration project, 2022-2025) held its kickoff meeting on 20 September. The project (part of the above-mentioned INNO-CCUS partnership) will capture CO2 at Aalborg Portland and Ørsted, comparing innovative solvents. Besides DTU Chemical Engineering and the industrial sites, the project partners are Union Engineering / Pentair, DTU Chemistry, Aalborg University and FORCE Technology. Project activities have already begun with the installation of a DTU $CO_2$ capture pilot at Aalborg Portland. Associate Professor Philip Fosbøl, DTU Chemical Engineering is project leader for this large project.

Associate Professor Wei Yan, DTU Chemistry, is project lead for the project CompReact—Compositional Simulation of Reactive Transport in $CO_2$ Storage, running from 2023-2026. The project will develop robust and efficient compositional geochemical simulation technology and integrate it with the open source GEOSX simulator. TotalEnergies, Noreco, and Ineos are the current industrial partners in the project.

Wei Yan will also participate in ThermoCO2Well, Risk Assessment of the $CO_2$ injection well damage due to thermal stresses running from January 2023 to September 2024. The project will build a numerical simulation model for $CO_2$ flow in the well, coupling flow and geomechanical effects. DTU will support the equilibrium calculation and thermodynamic properties in the study.

*Associate Professor Alexander Shapiro*

### 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
Union Engineering - 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.

# Pilot project "Greensand" in Danish North Sea

*Credit_INEOS Energy*

**The Danish Parliament decided in December 2020 to fund a Danish $CO_2$ storage pilot project named Greensand. The project aims to investigate the reservoir-$CO_2$ interaction in the Danish North Sea.**

Project Greensand is amongst the frontrunners of $CO_2$ storage projects in Europe. The project has the potential to make a significant contribution to our understanding and growth of carbon storage technology, whilst supporting Denmark's wider $CO_2$ emission reduction targets for 2030 and beyond.

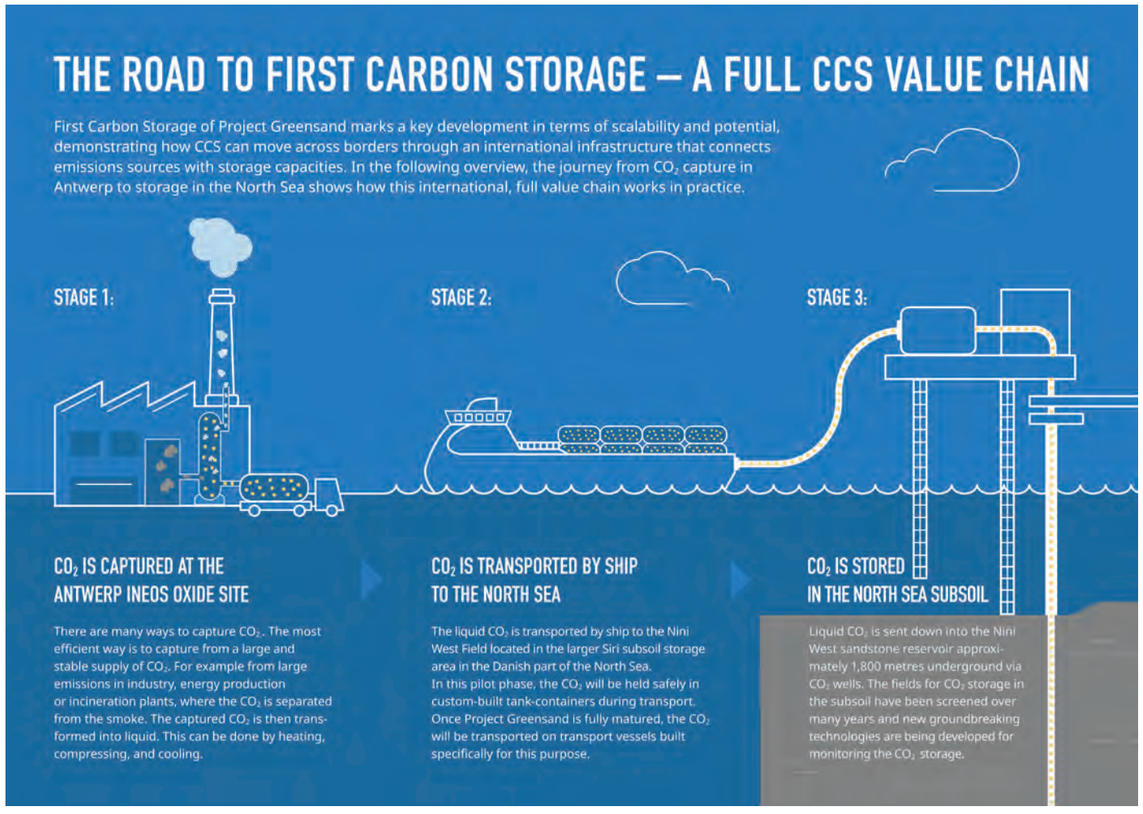
A consortium of 29 companies, research institutes and universities, have signed an agreement to support the Greensand pilot. The consortium comprises major Danish companies, international companies with expertise in carbon capture, international research institutes and universities, as well as small Danish start-ups with groundbreaking ideas on monitoring technologies.

Consortium members:

- Aalborg Portland
- Aker Carbon Capture ASA
- Blue Water Shipping
- DanUnity
- DFM
- DHI
- DTU
- Energy Cluster Denmark
- Esvagt
- Geelmuyden Kiese
- GEUS
- INEOS Energy (E&P A/S)
- INEOS Oxide Antwerp (INEOS NV)
- Maersk Drilling
- Magseis Fairfield
- Makeen Energy
- NLIR
- NOC
- Rambøll
- Resen Waves
- SAExploration
- Schlumberger - New Energy
- Semco Maritime
- Southampton University
- SpotLight
- Teknologisk Institut
- Welltec
- WindPowerLab
- Wintershall Dea.

*Associate Professor Wei Yan, CERE, has received funding through the Greensand project for investigation of the feasibility of $CO_2$ storage in certain underground chambers in the North Sea.*

The project targets the development of $CO_2$ storage capacity in the Danish part of the North Sea based on reusing discontinued offshore oil and gas fields for permanent $CO_2$ storage.
After successfully completing initial technical validation studies, Project Greensand recently received 197 MDKK from the Energy Technology Development and Demonstration Program (EUDP) via the Danish Energy Agency for phase 2.
As part of the project and phase 2, Wei Yan has been granted 3.9 MDKK.
"Our involvement is on the reservoir aspect. We will investigate what happens if a huge amount of $CO_2$ is injected into the underground storage site currently filled with brine and residual oil", says Wei Yan.
The contribution from the CERE research team is two-fold: First, they will measure fundamental thermophysical properties critical to the simulation of the multiphase flow involving $CO_2$, brine, and oil. Secondly, they will investigate specifically salt precipitation during injection of the large amount of $CO_2$.
"Our experimental and simulation study will reduce the risk of the injectivity impairment



due to salt precipitation", says Wei Yan.
The Greensand project aims to provide the basis for a decision to enable $CO_2$ storage by 2025.

**About Greensand**

- The primary objective of the Greensand project is to safely and permanently store potentially up to 8m tonnes of $CO_2$ per annum in the INEOS operated Siri area.

- The storage potential, if achieved, will contribute significantly to Denmark's 2030 overall emissions reduction target

- The Greensand project has three phases: Appraisal, Pilot (Proof of concept) and Full project execution.

- The Completed Appraisal phase had field owners INEOS, and Wintershall Dea, plus consortium members Maersk Drilling and GEUS.

- The project recently cleared a major hurdle as DNV GL independently certified that the Nini West field is conceptually suitable for injecting 0.45 million tons $CO_2$ per year per well for a 10-year period, and that the subsea reservoir can safely contain the $CO_2$.

- Pilot phase (Proof of concept) planning is now getting underway with potentially start around Q4 2021 subject to the implementation of the agreements outlined in the Danish North Sea Agreement of Dec. 2020.

- The The Final Investment Decision for the full-scale project will commence after proof of concept, planned in the second half of 2023, and will have an estimated delivery duration of around 24 months after which carbon storage could be operational from around 2025.

- The Paleocene sandstone fields of the Siri Area in the Danish North Sea are located at an optimal depth of 1.5-2.2 km and are encased in one of the most competent cap rocks in the North Sea. The area is geologically extremely stable and has retained gas and oil for 10-20 million years, the area constitutes a very safe permanent storage site for $CO_2$.

- In Phase 1, the Greensand Consortium demonstrated that viability of the development of a $CO_2$ storage site. The assessment was certified by DNV. The Storage potential is ½-1 million ton of $CO_2$ per year from 2025, increasing to 4-8 million tons of $CO_2$ per year by 2030. Hence, the Greensand Area can account for all the $CO_2$ storage proposed in the Danish Climate Program.

*Associate Professor Wei Yan*

*Credit_INEOS Energy*

# Green carbon capture receives funding


*Electrochemical carbon capture set-up at Vandcenter Syd*

A new project named Green Carbon Capture and Hydrogen production (CCCH2) will develop a carbon capture technology based on electrochemical regeneration of the solvent combined with hydrogen production. The technology will be demonstrated together with project partners Estech (lead partner), PureteQ, VandCenter Syd and Dansk Gasteknisk Center A/S.

The project has received 33 million DKK from the EUDP program of the Danish Energy Agency. Hereof, 4.7 million DKK are allocated to CERE. Associate Professor Philip L. Fosbøl and Senior Project Manager Sebastian Villadsen represent CERE in the project.

The project will run for three years and will support a postdoc, a PhD student and technical personnel.

The goal of the project is to demonstrate that the technology is scalable going from 10 kg $CO_2$/h removal (pilot scale) to 100 kg $CO_2$/h removal from the flue gas (demonstration scale), meeting two key objectives:

- Scale up the technology to demonstration size, where process parameters and CAPEX/OPEX can be evaluated.

- Demonstrate the reliability and the robustness of the technology and make it ready for commercialization.

Once these objectives are met in this proposed project, the technology must be matured including scaling from 100 kg/h $CO_2$ removal in this project to full-size plant.

Estech has devised a process in which carbon is captured from flue gas using a solvent that is regenerated using (green) electricity in an electrochemical process and generates hydrogen that can be converted to other energy forms (Power-to-X), thereby delivering both carbon capture and Power-to-X solutions at the same time. The process is expected to be energy neutral and if the hydrogen is sold at current market values, the carbon capture will be free.

*Pictures by Tessa Lund Biel-Nielsen*

*Ph.D Student Maria Dimitriadi Performing gas composition measurements for carbon capture*

Waste and biomass valorization

*Associate Professor Hariklia Gavala*

# A summit of green engineering

*Conference dinner at restaurant "Grøften", Tivoli*

**In 2022, CERE had the honor of hosting the world's leading conference on waste and biomass valorization.**

Initiated in 2005, the bi-annual WasteEng has evolved into the world's leading conference series on waste and biomass valorization. Venues change, with CERE and DTU Chemical and Biochemical Engineering hosting in 2022.

"Since we began the conference series, we have gradually seen a change in perspective. Back then it was very much about the technologies. Having a given waste fraction, which products would we be able to convert it into – energy, chemicals, materials. Today, we more often start with addressing the usage. This is a completely different approach. I do believe that innovation is more likely to succeed when you take market demands as your starting point," says Ange Nzihou, Professor of Chemical Engineering at Institut Mines Telecom, Mines Albi, France. Professor Nzihou is the Founding chair of the WasteEng conference series.

*Ange Nzihou. Professor of Chemical Engineering at Institut Mines Telecom, Mines Albi, France.*

Due to the depletion of natural resources, transition into a green economy is a given task, Ange Nzihou continues:

"My message would be that this is not only necessary, but also possible. Most of the goods we need can for example be produced from biomass. Of course, production of food should be the top priority, but even after this demand is met it will be possible to have enough renewable raw materials to produce energy, chemicals, and materials. And notably, we may even improve the properties of some materials as we apply renewable feedstocks."

**An extended scientific family**

Associate Professor Hariklia Gavala, CERE, co-organized WasteEng2022, and was key coordinator for the

conference at DTU.

""The WasteEng conference series marks 17 years of breakthrough research and

*Associate Professor Hariklia Gavala*

innovation in waste and biomass valorization. Based on 435 submitted abstracts, some 350 oral and poster presentations were provided during the WasteEng2022 conference, showing the richness of this ever-growing field," says Hariklia Gavala, adding:

"The presentations contribute significantly to the promotion of sustainable valorization of waste and biomass to produce energy and useful materials, with emphasis on processes and practices that reduce emissions and life cycle assessment of technologies and end-of-pipe products. Moreover, in WasteEng I always enjoy the atmosphere that brings with and the feeling of belonging to an extended scientific family – for all these reasons I was very happy to be the local organizer of WasteEng2022."

## A truly global format

To encourage participation from developing countries, the WasteEng organizers have set up a mechanism. Scientists from developing countries will submit abstracts, and the organizers will award the best entries with grants allowing them to participate. The mechanism is based on funding from the European Union and industry.

Professor Animesh Dutta is Director of the Bio-Renewable Innovation Lab, University of Guelph, Canada. He is a fan of

*Professor Animesh Dutta*

the scheme for attracting talents from developing countries:

"What I like most about WasteEng is the global perspective. I do attend other conferences, mainly in either North America or Asia. Normally the focus of these conferences would be the continent where the event is held. While WasteEng is a European conference, only some 50 per cent of the participants are European."

Due to the COVID-19 pandemic, WasteEng was held online in 2020. Animesh Dudda prefers the physical format, he admits:

"The conference discusses research results, as well as applications that focuses on cutting-edge R&D and addressing barriers related to the chemical, bio-chemical and thermo-chemical conversion of biomass, co-products and bio-waste into fuels, energy to added-value materials. Being a top-tier research university in biomass and waste conversion, DTU is an ideal place to re-start the WasteEng conference series physically after a long four years."

## Every third space reserved for young talent

Some years ago, as the WasteEng series became ever more popular, the organizers decided to set a ceiling of 400 participants. The aim is to have 60 per cent familiar faces and 40 per cent newcomers. Further, one third of the spaces are reserved for young talents, meaning either PhD or Master students.

*PhD student Ekaterina Korotenko*

One young participant is Ekaterina Korotenko, PhD student at the University of Chemistry and Technology, Prague, Czech Republic.
"What can I say. I love waste!" Ekaterina Korotenko contributes to the scientific content of the conference with a presentation on valorization of one of the trickiest types of waste: bottom ash from solid waste incineration.

"Fly ashes from incineration do contain many valuable fractions. My presentation today will focus on valorization of salts in the ash. In other projects we focus on metals and on minerals which can be useful in the construction industry," says Ekaterina Korotenko, adding:

"In all these contexts several pollutants in the resulting products can be problematic. So, you can look at what we do either as trying to solve hazardous waste problems, or as finding valuable resources. Both are true, it depends on the point of view."

*Professor Lisbeth Olsson*

## Focus on solutions with application

Lisbeth Olsson, Professor in Industrial Biotechnology, Chalmers University of Technology, Sweden, attends the WasteEng conference for the first time.

"I am a regular participant at an international conference – Symposium on Biomaterials, Fuels and Chemicals - which is held annually in USA. Still, I feel it is also important to get a European perspective."

To illustrate her point on the challenges of waste engineering, Lisbeth Olsson compares with petrochemical engineering:

"Fossil oil is pretty much the same regardless of the country where it is produced. In waste valorization, you face very different challenges if you want to process, say, organic waste from production of olive oil, or residues from production of alcohol. Therefore, waste valorization very often has a geographical dimension."

"At the same time, it becomes increasingly important in waste valorization to work across disciplines. WasteEng is more holistic than many other conferences. You don't get very deep into details of specific technologies. Instead, there is a strong focus on developing solutions which can be applied."

"Also, I am pleased to see a large contingent of young participants. Especially after the pandemic, it is nice to see that young researchers can attend physical events again and build networks."

## We need to reinvent our technologies

*Professor Gerasimos Lyberatos*

Professor Gerasimos Lyberatos, Director, Organic Chemical Technology Laboratory, National Technical University of Athens, is a member of the scientific committee for WasteEng2022.
"What I like about the format is that it is not too specialized. A wide range of technologies are represented, for example biological, thermochemical, and catalytic transformation techniques. Often these fields would have their own dedicated conferences. Here, all are represented. This allows for contacts across the different fields, and for discussions on possible hybrid solutions."

Now is an exciting time to work in waste and biomass valorization, Professor Lyberatos argues:

"More than ever has it become evident, that what we do meet societal needs. For instance, climate change and lack of energy resources are two driving factors. Being a chemical engineer, I feel a shift in the focus. During the 20th century, we developed a range of technologies which helped in making everyday life easier. Plastics, just to name one example. Now we face the next big challenge. If the modern lifestyle is to be maintained in a sustainable way, we need to reinvent all our technologies."

"For a long time, we have been operating a linear economy. Goods were produced, and later dumped as waste. 30 years ago, the focus was on how to dispose of this waste in a safe manner. Today, we want to create a circular economy. What we do has a dual purpose. We want to bring down the amounts of waste, but we also want to create new resources. Hopefully, the word "waste" will soon become redundant!"

## Different routes to valorization

Another member of the scientific committee for WasteEng2022 is Professor Laurence Le Coq, Dean for Research & Innovation, IMT Atlantique, France:

*Professor Laurence Le Coq*

"Being a chemical engineer working in thermochemical conversion, I feel it important to meet researchers in other technology fields. Surely, the thermochemical route is not the only way to achieve valorization of waste. Here, I can meet researchers working in enzymatic, microbial, catalytic, and other routes. It is healthy to have an open mind as to which route will be best suited for a given task. Sometimes the best way forward is to combine different technologies. Tools such as life cycle assessment may aid in this process. A good starting point will always be to take a broad approach to the problem at hand rather than having chosen at technology beforehand. The strength of WasteEng is the way the different research communities are mixed."

At IMT Atlantique, Professor Le Coq is already involved in interdisciplinary research.

"However, not all my colleagues work on waste. Therefore, it is good to attend a conference where everybody focusses on waste valorization. I often see some use cases which are relevant to bring home."

"I have attended all conferences in the series. People here are used to communicate, and many of us know each other well. This makes it easy to discuss new ideas and possible joint projects. Still, I would like to stress that we are not a closed circle. To the contrary, I would argue that way we veterans have bonded over the years makes things easier for newcomers. You may ask any of us and you will be directed to somebody who can answer your question."

*Conference dinner at restaurant "Grøften", Tivoli*

*Professor Gregory Stephanopoulos*

## A hands-on scientific community

Professor Gregory (Greg) Stephanopoulos, Professor of Chemical Engineering and Biotechnology, MIT, attends WasteEng for the first time.

"It is interesting for me, coming from the biological side, to attend a conference with so many approaches present. The scientific content ranges all the way from the molecular level to which types of feedstocks to utilize."

"Moreover, the full range of valorization is covered. In one end of the specter, you have high-value products such as pharmaceuticals where the cost of the feedstock is close to

insignificant, and in the opposite end you have fuels and commodity chemicals which are very sensitive to cost. While high-value and low-value applications are very different in nature, both types of valorizations are relevant – and addressed at WasteEng."

Further, Professor Stephanopoulos makes a distinction based on the composure of the waste:

"For solid types of waste materials, you will normally have mechanical or thermochemical treatment, which is not my domain. For the softer types – food waste, certain polymers etc. – microbial treatment is an obvious choice. The main challenge lies in how to engineer the microbes, so they become optimal for the product you want. Finally, we have the gases. Carbon dioxide is very much in focus. Here, the problem is how to make this inert gas accessible for further processing into useful products. The attention right now is on reactions with hydrogen."

"Compared to your average biotech conference, I find WasteEng to be very hands-on," he comments, adding with a smile:

"I almost get the feeling that some of my fellow participants might go the DTU cafeteria at any moment, ask for some waste and start an experiment. Okay, that might be an exaggeration, but my point is that people here want to see results in the real world. They will not hesitate to go to the local municipal waste treatment facility to get the raw materials they need for their research."

WasteEng2022 was held at DTU June 27-30, 2022.

# Gas processing

*Ph.D. Student Julia Trancoso Fernandes dos Santos*



# Thermodynamic modeling as basis for the digitalization of gas processing


*Ph.D. Student Julia Trancoso Fernandes dos Santos and Professor Nicolas von Solms*

## Especially for subsea applications, accurate prediction of gas processing behavior is extremely important at Equinor.

CERE Ph.D. student Julia Trancoso Fernandes do Santos connects for the online interview from the Equinor research center in Trondheim, Norway. "The level of digitization at Equinor is advanced. We can get online data from real gas processing around the clock and compare it to the values predicted by the digital twin. As soon as the model is truthful enough, it has many applications, as predictive maintenance, for example."

The collaboration with Equinor began more than 20 years ago, when Georgios Kontogeorgis, today Professor in CERE, developed the Cubic Plus Association (CPA) thermodynamic model. Most of the work has been under the umbrella of the CHIGP (Chemicals for Gas Processing) Joint Industry Project. In total, six PhD projects have been sponsored by the Norwegian energy corporation, with Julia's project as the most recent.

Dr. Even Solbraa at Equinor has been the industry contact for most of those projects.

Originally, the main goal of the collaboration was to minimize the amounts of chemicals used in gas processing, for instance glycols which are used as hydrate formation inhibitors. Lower use of additives equals less environmental impact, and also lower costs. Further, added chemicals will later have to be removed from the gas stream to meet specifications. Thus, every reduction in use of chemicals is in fact a double saving since less energy need to be used at the later removal stage.

### Optimizing the set of parameters

Currently, the glycol of choice in this type of gas processing is TEG (triethylene glycol).

"When I joined CERE to start my project a-year-and-a-half ago, the environmental goals in terms of TEG emissions at Equinor were already achieved, but we could still see some small losses into the gas phase, which we've been trying to optimize even further" says Julia Trancoso Fernandes do Santos.

The CPA has proven useful beyond the original scope, she explains:

"Right now, our main focus is to improve the parameters of our thermodynamic model. The real process data and the TEG losses predicted by our model are not in agreement. With a new optimized parameters set, we can check if the model was the problem or if there is something else wrong in the process, improving the regeneration of TEG."

Process behavior prediction is especially important in relation to subsea gas processing. An increasing share of Equinor's gas production comes from subsea wells.

**Why subsea processing is desirable**

The traditional solution of transporting a mixture of water and gas to an onshore processing plant has significant drawbacks.

Firstly, the length of the pipeline is constrained due to the risk of problems such as slugging and gas hydrate formation. By instead transporting pure gas, these problems are minimized. So, the pipeline can be much longer, meaning resources further away from a central treatment facility can be reached.

Secondly, subsea processing saves energy. In the deep reservoirs, the gas is under high pressure. This is handy in respect to removal of water. Under high pressure, the water will tend to separate without any further measures. But if you – as traditionally seen – transport unprocessed gas over several kilometers, the pressure will drop. You will need to either invest energy in getting the pressure up again, or use intensified processing, also requiring energy consumption. By removing water at the well, the original pressure can be utilized.

Thirdly, dehydrating the gas at the sea floor reduces the need for addition of chemicals such as TEG. In traditional offshore recovery, chemicals are added for gas hydrate inhibition to prevent pipe blockages leading to serious downtime.

However, operating gas processing subsea does involve challenges such operate unmanned facilities, common in this type of process, which with the digitalization can be done at Equinor remotely.

*Ph.D. student Julia Trancoso Fernandes dos Santos*

**From Curitiba to Trondheim**

Julia Trancoso Fernandes do Santos is half-way through her Ph.D. project. Following 14 months at CERE in Denmark, she completed a six-month stay with Equinor, working with Dr. Even Solbraa

Asked how she has adapted to the change from Denmark to Norway, Julia strikes a diplomatic note:

"As a Brazilian, I see a lot of similarities. Both in Copenhagen and in Trondheim I found people to be extremely friendly. Well, of course the mountains here make a big difference in the scenery. Also, I arrived at Christmas time, meaning a lot of traditional parties."

Julia took her master's in chemical engineering in her home city of Curitiba, the 8th largest city in Brazil, with roughly 2 million inhabitants.

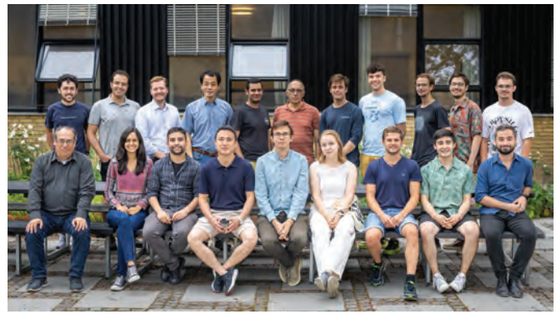
"So, it was a big change to arrive here in Trondheim – the third largest city in Norway, but a very small place if you come from Curitiba," Julia smiles.

More importantly, though, the Ph.D. project has opened the door to a change of career:

"In Brazil, I was working in industry, but I always felt more attracted to academia. So, this is a dream come true for me!"

# NEWS FROM CERE

## Revival of the Thermodynamic Models Course



*Group picture of CERE summer course on advanced thermodynamic modelling*

During COVID lockdowns, the traditional CERE summer course on advanced thermodynamic modelling was held online but in 2022, the course was again given in person.

Participants from Kyrgyzstan, France, United Kingdom, The Netherlands, China, Chile, Lebanon, Brazil, and Denmark attended. Two participants kindly share their impressions of the two weeks course:

Gustavo Chaparro, PhD student at Imperial College London:

"I feel like I learned a lot from this summer school. The expertise from DTU in thermodynamics is unquestionable. Also, I got to familiarize myself with the Danish culture and to explore Copenhagen and Lyngby. I appreciate opportunities like this as I am originally from Chile, and we don't often get the chance to come to Denmark. Finally, I am glad to get to know other students in the field. We shared a lot of moments, some of frustration, for example, when our code didn't work but also moments of joy. We shared lunches, we went out and even got to join the summer party from the chemical engineering department, which was much fun too! Well, I can only say good things about this experience. I will definitely recommend the school to other students!"

Michiel Wapperom, PhD student at TU in Delft, The Netherlands:

"I enjoyed two great weeks of summer in Copenhagen. The weather was extraordinarily good, and we spent long days at the university. The mornings were dedicated to lectures covering a particularly broad range of topics in thermodynamics. Mr. Yan gave an in-depth insight into computational aspects, Mr. Kontogeorgis passionately showed us his world of thermodynamic models, Mr. Shapiro took a more fundamental approach in thermodynamic modeling, and Mr. Fosbøl connected all the previously mentioned topics into some very relevant industrial applications. The afternoon exercise sessions were short for some, long for others. Even though two weeks of being a student again was challenging and intense, we managed to meet great people and have some time off."

## Postdoc grant for hydrate research

CERE Postdoc researcher Jyoti Shanker Panday

*Postdoc Jyoti Shanker Panday*

has received a prestigious grant from Independent Research Fund Denmark for gas hydrate studies.

Improved hydrate technology should help capture and store both $CO_2$ and hydrogen.

Denmark has set a target of 70 % greenhouse gas emissions by 2070 compared to 1990. To achieve this ambitious goal there is an urgent need to develop carbon capture technologies, and to develop storage technologies for both $CO_2$ and hydrogen. Gas hydrate technology could be a platform for both purposes.

Gas hydrates are ice-like crystalline compounds that can store gases such as $CH_4$ (methane), $CO_2$, and $H_2$ (hydrogen). Hydrate-based technology is cost-effective, non-hazardous, and environmentally friendly compared with competing technologies. However, hydrate technology is immature because of slow kinetics and low gas storage value.

The project aims to improve the kinetics of hydrate formation by introducing 3D porous metal-organic frameworks. According to the underlying hypothesis, the critical properties of the metal organic framework, such as the large surface area and high gas selectivity, would lead to a significant improvement.

The funding from Independent Research Fund Denmark is provided under the International Postdoc Fellowship Grant. Jyoti Shanker Panday and colleagues at CERE will carry out fundamental research on the application of MOFs in hydrate technology.

**Looking at the intriguing properties of water**

While much is known about the structure and properties of water, many of its properties are anomalous in the sense that no other liquids behave like this. Supervised by Professor Georgios Kontogeorgis and Associate Professor Xiaodong Liang, a new Postdoc researcher will be recruited for fundamental water studies in CERE.

Many of the anomalous properties of water are of thermodynamic origin. Examples are density maximum and minimum heat capacity with respect to temperature. It has been known as a concept for over a century that water may consist of two states in some form of mutual equilibrium. But only during the last 20 years has this theory regained serious attention through advanced experimental, simulation, and theoretical studies. Currently, even the most advanced thermodynamic models are incapable of simultaneously capturing the anomalies of water and complex phase equilibria of water containing systems.

The goal of the project is to investigate whether the combination of the two-state concept and advanced thermodynamic models based on the SAFT framework can describe the anomalous properties of water.

The new project is made possible by a Villum Experiment grant from the Villum Foundation.

**Soil remediation by salinity waves**

Can brines with different salinities be utilized to remediate soil from colloidal contaminants such as plastic particles? Postdoc researcher Tian Wang, CERE, has received a grant from

*Postdoc Tian Wang*

the Villum Foundation to investigate this topic.

The idea is to use the salinity waves – alternating high and low salinity, or high-low-high concentrations of specific ions. It is expected to be a simple, cost-effective, and energy-saving method, which can minimize the overall environmental impact of soil treatment. The fact that the particles can move in the capillaries under the action of varying salinity has previously been confirmed in microfluidics experiments. The new experimental program aims to verify the possibility of cleaning soil from multiple contaminants. The experiments will be performed with application of both 2D and 3D microfluidics, on glass beads and sand packs.

Tian Wang will work with Assosiate Professor Alexander Shapiro, CERE and Professor Simon Andersen, Danish Offshore Technology Center. The project has received a donation of 2 million DKK under the Villum Experiment program.

**Poster award for thermodynamics research**

Ph.D. student in CERE Gabriel Moraes Silva received the Helmut Knapp Poster Award


*Ph.D Student Gabriel Moraes Silva*

at the ESAT (European Symposium on Applied Thermodynamics) conference in Graz, Austria, July 2022. The honor was based on his work entitled "The specificities of the different deviations of the Dybye-Hückel equations." The content was also published in the Molecular Physics Journal.

Gabriel Moraes Silva initiated his Ph.D. project "Modelling of Electrolyte Systems using the Non-Primitive Approach" in November 2021, supervised by Professor Georgios Kontogeorgis and Associate Professor Xiaodong Liang. The project is funded by the European Research Council (ERC) Advanced Grant "New Paradigm in Electrolyte Thermodynamics".

**Students visit Maersk Resolve jack-up rig**

Members of the Society of Petroleum Engineers (SPE) Copenhagen's student chapter were given the opportunity to visit the Maersk Resolve jack-up rig at Esbjerg Port.

The rig is 150 meter tall and capable of hosting a crew of 130 with a galley (kitchen), gym, cinema, and a helicopter landing pad. The rig must be self-sustainable during operation and is equipped with a 2.4 GW generator that delivers electricity for heating, drilling, ventilation, and desalination of 120 tons of water daily.

Maersk Resolve can drill at water depths of up to 106 meters, and drill wells up to 10,668 meters.

The excursion was made possible by funding from DTU Chemical and Biochemical Engineering.

**Leading expert in $CO_2$ storage lectures**


*Yu-Shu Wu*

The ongoing efforts in CERE within carbon capture and storage received additional inspiration as a world-leading researcher in $CO_2$ storage, Yu-Shu Wu of the Colorado School of Mines (CSM), USA, visited on June 23, 2022. Yu-Shu Wu is a professor in petroleum engineering and Director of the Energy Modeling Group at CSM.

In his presentation, Professor Wu discussed multi-physical processes involved in CO2 geo-sequestration and the research made at the Energy Modeling Group to develop quantitative modeling tools for the field. Specifically, an advanced reservoir simulator, TOUGH2-CSM, was introduced to the CERE staff. The simulator can model CO2 storage under thermal-hydrologic-mechanical or thermal-hydrologic-mechanical-chemical effects in saline aquifers. Professor Wu showed several application examples where the simulator was used.

**Strong presence at conference on capture**

A full dozen CERE researchers participated in the greenhouse gas control technologies conference GHGT-16 in Lyon, France, October 2022.

The focus of the GHGT conference is to acknowledge the importance of carbon capture, utilization, and storage (CCUS) to reduce $CO_2$ emissions and meet the Paris Agreement. CERE participated with 3 oral presentations and 10 posters.

The CERE presentations highlighted results from the projects 3D, BioCO2, Consen-CUS, Net Zero Energy Carbon Capture at Amager Resource Center: pilot scale development and demonstration of carbon capture from waste-to-energy plants project which included pilot testing, solvent degradation, and SLE. CERE also presented scaling, and new process principles for $CO_2$ capture.

Further, CERE had two oral presentations on storage. One on simulation compositional, reactive transport for geochemical systems. And another on Enhanced Oil Recovery by gas injection in the lower Cretaceous reservoirs in Denmark.

The GHGT-16 conference had 1,100 attendees.

# PhD Theses

Einar Madsen Storebø, Ph.D.

# Effect of pyrite on fluid distribution and permeability modelling of North Sea Lower Cretaceous clay rich carbonate reservoirs.

Supervisor: Professor Ida L. Fabricius.

*The project was funded by the Danish Hydrocarbon Research and Technology Center. (Now Danish Offshore Technology Centre) as part of its Lower Cretaceous program*

## Permeability of deep North Sea carbonate reservoirs

In the Danish sector of the North Sea, hydrocarbon reservoirs have been found in two distinct carbonate successions: the well-understood and extensively researched Upper Cretaceous and Cenozoic chalks and the deeper, lesser-explored Lower Cretaceous marly chalks. In the project, borehole-geophysical methods for establishing fluid distribution and modelling permeability of North Sea Lower Cretaceous carbonate reservoirs were developed.

Lower Cretaceous chalk layers in the Central Graben in the Danish part of the North Sea contain substantial oil and gas reserves, but also a varying content of clay, which lowers oil flow, so these reservoirs have till date been underdeveloped.

For two Lower Cretaceous formations, Sola (Upper Barremian-Lower Albian) and Tuxen (Upper Hauterivian-Barremian), a regional stratigraphic framework exists (Ineson, 1993) with Sola categorized as a heterogeneous stratigraphic unit of marl and claystones, and Tuxen as a bioturbated coccolith chalk interbedded with faintly laminated marlstone. Within the Tuxen and Sola formations disseminated pyrite is present but not obviously prevalent, so its significance as an electrical conductor has been overlooked. Pyrite ($FeS_2$) is an iron sulfide commonly found in sedimentary rocks. In the project, a methodology for evaluation of water saturation in clay-rich carbonates with measurable amounts of pyrite was provided.

Four approaches to model permeability in clay-rich carbonates from well log data were calibrated to core plug measurements. The use of these four methods was demonstrated in the Lower Sola, Upper Tuxen, Middle Tuxen, and Lower Tuxen formations in the well Boje-2C obtaining the petrophysical values and fitting parameters needed for accurately determining permeability accordingly. Porosity is normally well established from well log data, so the challenging task is to find the friction-giving specific surface.

For the studied formations, all four methods produce a good fit to measured permeability, when the correct fitting values are used: 1) For the spectral gamma ray, the specific surface used for permeability calculation can be found by correlation; 2) To obtain permeability from water saturation, the modelled water film thickness must be adjusted by a formation-based multiplier; 3) Nuclear magnetic resonance surface relaxivity can model permeability without any additional fitting parameters also in hydrocarbon bearing intervals; 4) The use of flow zone indicators resulted in four distinct formation-based linear relationships between compressional wave velocity and permeability, indicating each formation belongs to its own separate hydraulic unit.



Lisa Pasquinelli, Ph.D.

# Heat Storage in Hot Aquifers – the feasibility of high temperature aquifer thermal energy storage in Denmark, the Gassum Formation in the Stenlille Structure.

**Supervisors: Professor Ida L. Fabricius and Professor Klaus Mosegaard.**

*The project was sponsored by the Danish Council for Strategic Research as part of the HeHo (Heat Storage in Hot Aquifers) project developed in collaboration with GEUS, Dansk Fjernvarmes Geotermiselskab, and the Niels Bohr Institute.*

## Heat storage in hot aquifers

The ability to store excess energy will be key for transition into a non-fossil future powered by renewable but fluctuating energy sources. High-Temperature Aquifer Thermal Energy Storage (HT-ATES) is a promising heat storage technology. In the project, modeling of a Danish geological structure feasible for HT-ATES was developed.

Heat storage technology could contribute to reducing greenhouse gas emissions by storing excess energy from waste incineration, solar panels, biomass plants, industrial processes, and windmills. Integrated with new geothermal plants, HT-ATES allows minimal heat loss and large storage capacity. Specifically for Denmark, HT-ATES is likely to be the missing link in planning sustainable energy production.

A typical scenario would involve seasonal cycling: the deep (hot) aquifer is penetrated by wells; in winter, cold water from a heat exchanger is injected into the cold wells, while warm water from the aquifer is extracted from the warm wells; in summer the pattern is reversed, and heat is stored in the aquifer by injection of heated formation water of 75-200 °C.

HT-ATES is particularly interesting in Denmark, where several sandstone reservoirs may be suitable. However, while heat storage in the Danish subsurface is gaining increasing interest, no deep heat storage facilities have yet been established. The project aims to discuss which geological and technical characteristics should be present for a heat storage reservoir in Denmark. The Gassum Formation in the Stenlille structure was chosen as the subject for developing a model. This formation is presently used for gas storage, and a range of data are therefore already known.
A 2D model ("the Simple Model") and a 3D model ("The Stenlille Model") for a HT-ATES system were developed using analysis of geological data and geophysical data such as core data, well logs, and seismic lines. Further, heat transfer and finite elements were utilized to calculate recovery efficiency, heat storage capacity, and thermal breakthrough time.
In the Simple Model, a simplified geological model of the Stenlille structure is used, and in the Stenlille Model, the Gassum Formation is modelled in three scenarios according to real data and combinations of different data sources with the use of geo-statistics. Both models are feasible and lead to similar results.

Based on geostatistical methods, a high recovery efficiency of 72 % was found. Further, the heat storage capacity proved high (1.8 x 1018 J). Finally, the ability to store heat over time – measured as the thermal breakthrough time - was long; 66-77 years.

Mick Emil Kolster, Ph.D.

# Drone-based scalar magnetic surveying for unexploded ordnance and geological applications.

**Supervisors: Senior Researcher Arne Døssing Andreasen and Professor Nils Olsen.**

*Funding was provided by Innovation Fund Denmark.*

## Drone systems for unexploded ordnance detection

Unexploded bombs and mines from past wars constitute a major risk factor in relation to offshore activities such as construction and maintenance of wind energy farms and other installations. In the project, magnetic surveying by drone was employed and shown to be an effective method for detecting unexploded ordnance (UXO).

Earth's naturally occurring magnetic field interacts strongly with metallic objects such as UXO. Therefore, towing magnetometers from drones has the potential to be a both efficient and relatively cheap way to identify UXO at the sea bottom. Magnetic measurements will not show the metallic objects directly, but their positions can be derived through inversion. In the project, a source inversion strategy based on finite differences was developed.

Detection tests performed across a variety of UXO targets found that the inversion scheme can provide three-dimensional positioning estimates sufficient for practical recovery of UXO. The inversion method was extended to include erroneous time shifts between measured scalar field data and recorded sensor positions. Subsequent correction of survey data suffering from such shifts yielded actionable target position estimates for various targets, ranging from a 0.5 kg hand grenade to a ~24.5 kg, 155 mm artillery shell.

UXO detection and inversion was studied across several flight altitudes, in different settings, using different sensor configurations, and across 50 different unexploded ordnance and scrap objects. According to the studies, ferrous objects of less than 10 kg can routinely be detected with a slow-moving vertical magnetic gradiometer system, with detection and accurate positioning of objects as small as ~500 g documented from altitudes of ~2 m in a tidal flat, based on a data line spacing of 50 cm. Larger UXO targets were found to be readily detectable at higher altitudes, and with larger line spacings, as demonstrated with a high-speed (> 10 m/s) multi-sensor bird system, which was found to constitute an efficient survey approach for larger UXO targets in the tidal flat setting. A joint inversion across all three sensors enabled modeling and subsequent removal of 50 Hz power line noise signals with amplitudes below ±5 picoTesla from the measured scalar magnetic data, providing strong testimony to the potential of pairing present-day Optically Pumped Magnetometers with the drone-towed approach.

Apart from UXO applications, consideration was given to mapping of larger-scale geological features, where a dual scalar magnetometer bird with horizontally aligned sensors was applied in a mineral prospecting setting and compared to ground survey data collected in the same area. The ability of low altitude flight with close terrain following was found to provide data with a high correlation to traditional ground surveys, while retaining an estimated dynamic response level on the order of tens of picoTesla. The data, which was obtained by draping the survey lines across the topography, provided a high resolution that enable detection of subtle geological features. The obtained results suggest that drone-based surveying is superior to ground surveys in many settings, due to a combination of improved data quality, coverage ability, and coverage rate. Furthermore, it is argued that drone surveys may provide a suitable alternative to helicopter-borne surveys at a fraction of the price.



Mark David Wigh, PhD.

# A probabilistic and machine-learning geophysical approach for characterizing potential Unexploded Ordnance.

**Supervisors: Senior Researcher Arne Døssing Andreasen and Associate Professor Thomas Mejer Hansen.**

*Funded partly by Ørsted A/S.*

## Identifying unexploded ordnance from magnetic data

Unexploded ordnance (UXO) such as ammunition, bombs, and mines represent both a safety hazard and an economic burden for laying of cables, building of offshore wind power facilities, and other constructive activities in the marine environment. To make matters worse, it is hard to distinguish UXO from other types of metallic objects at the seabed. Therefore, all objects need to be treated as if they were UXO. The project is a first step towards a methodology which may distinguish UXO from non-UXO objects based on data from magnetic surveys.

Past wars are the main source of UXO. The North Sea is contaminated with many kinds of UXO with the vast majority originating from World War II. At the same time, the seabed is contaminated with a large amount of other manufactured steel/iron objects. These non-UXO objects exceed the amount of UXO significantly, but since no reliable method of distinction based on remote sensing exists, all metallic objects must be carefully inspected under strict safety precautions, greatly adding to costs. The project was carried out in cooperation with Ørsted A/S.

The energy corporation needs to deal with the issues relating to UXO before the construction of its offshore wind farms. Total-field magnetometry using aerial drones or marine underwater towed vehicles is commonly applied in geophysics and is an efficient and relatively low-cost method. However, magnetic detection of UXO is often only a precursor for more expensive inspections, since inferring shape, size, and orientation from a magnetic anomaly is difficult. In addition, remanent magnetization in ferromagnetic materials causes further uncertainties.

In the project, inversion of the magnetic anomalies was carried out using a probabilistic approach, where the model parameters of interest are inferred as distributions in a stochastic simulation using Markov Chain Monte Carlo algorithms. Conceptual models of magnetized spheroids and rectangular prisms are used to simulate magnetic anomalies for the purpose of discriminating between UXO and non-UXO sources. The chosen inversion methodology has been tested on magnetic anomalies measured from drone as well as marine magnetic underwater surveys.

The probabilistic inversion approach was shown to be highly feasible as a tool for inferring magnetic anomalies. Remanent magnetization is a significant issue. By handling the unknown remanent magnetization in a probabilistic approach, the uncertainties related to discriminatory capabilities of UXO and non-UXO were addressed. The main findings indicate that remanent magnetization makes it very difficult to discriminate between shapes of ferromagnetic objects, due to high uncertainty. The remanent magnetization in UXO seems to have significant variations in strength as well as direction with respect to the object. When assuming high remanent magnetization strength in sources, no discrimination is possible between the conceptual models of prism and spheroids, but when reducing the remanence, some discriminatory capabilities seen likely. However, this is at the cost of possible false target classifications, which are expected to be caused by presence of high remanent magnetism not accounted for.

Fernando de Azevedo Medeiros, PhD.

# Chemical and Phase Equilibrium Simulation Tools for Underground Geological Storage of $CO_2$

**Supervisors: Associate Professor Wei Yan and Professor Erling H. Stenby.**

*Funded by DTU Chemistry*

## Forecasting $CO_2$ behavior in geological storage

Underground geological storage of $CO_2$ is widely regarded as necessary to control climate change. However, deployment in industrial scale relies on the development of tools capable of forecasting the long-term behavior of the injected $CO_2$. In the project, novel tools for this purpose were developed.

Injection of $CO_2$ in mineral formations may trigger numerous physical and chemical phenomena, which makes simulation of $CO_2$ behavior extremely challenging. For instance, simulators need to account for fluid flow in porous media, adsorption of certain components, phase splitting of components, and chemical reactions. Therefore, algorithms for chemical and phase equilibrium (CPE) calculations are key.

In the project, novel numerical simulations tools for $CO_2$ behavior in saline aquifers have been developed. All these tools are based on the RAND method which is a non-stoichiometric Gibbs energy minimization algorithm. The ability to handle chemical and phase equilibrium simultaneously gives the RAND method several advantages over the methods used in popular geochemical simulators.

The contributions in the project are both of theoretical nature, by expanding the general theory of CPE algorithm, and of practical nature, by applying the new findings to CO2 underground geological storage.

For the theoretical part, new types of CPE calculations were developed. Michelsen's two-phase flash framework for non-reactive systems was extended to open systems with fixed chemical potentials. The RAND method was then used as the counterpart of this methodology to reactive systems. In addition, a novel saturation point calculation method for reactive systems was developed. This algorithm was used to automatically generate phase boundaries and quality lines of reactive mixtures in many systems.

For the practical part, the path of certain mineral reactions was studied in scenarios of interest to $CO_2$ underground geological storage, e.g., by using the newly developed open flash algorithms. In addition, insights on salt clogging during $CO_2$ underground geological storage (risk of injectivity impairment in saline aquifers) were acquired through simulations coupling the RAND method with a 1D solver for flow in porous media. Finally, a fully implicit compositional simulator capable of simulating both reactive and non-reactive flow in porous media was developed with the RAND algorithm at its core.

Overall, the study has provided a basis for using the RAND method in various simulation analyses of $CO_2$ underground geological storage involving multiphase geochemical reactions, and the theoretical methods developed can potentially be applied to other reactive transport processes.

Arne Døssing Andreasen, DTU Space

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# Conference contributions & invited speakers

## JANUARY

**AAPG Europe workshop on CCS, online, 17-19 January 2022**

Ida L. Fabricius, Tobias Orlander, Anders Nermoen, "North Sea chalk: Carbon storage and Enhanced Oil Recovery", AAPG Europe workshop on CCS, online, 17-19 January 2022 (invited oral presentation + panel participation)

## FEBRUARY

**LOF lecture, Niels Bohr Institute, Copenhagen, Denmark 16 February 2022**

Michael Bache, "Molekylær vand forskning og vand omkring proteiner", LOF lecture, Niels Bohr Institute, Copenhagen, Denmark 16 February 2022 (Oral presentation)

**LOF lecture, Rønnebærhus Activity Center, Holte, Denmark, 17 February 2022**

Michael Bache, "Molekylær vand forskning og vand omkring proteiner", LOF lecture, Rønnebærhus Activity Center, Holte, Denmark, 17 February 2022 (Oral presentation)

## MARCH

**AAPG Carbon Capture, Utilization & Storage Conference, Houston, United States, 29-31 March 2022**

Tobias Orlander, Leonardo T. P. Meireles, Thomas G. Petersen, Ida Lykke Fabricius, Walter Wheeler, Roman Berenblyum, Anders Nermoen, Frederik P. Ditlevsen, "De-risking Danish large-scale CO2 injection into depleted chalk reservoirs", AAPG Carbon Capture, Utilization & Storage Conference, Houston United States, 29-31 March 2022 (Poster Presentation)

## MAY

**EUBCE 30th, online, 9-12 May, 2022**

Sebastian Borgquist, Sebastian N. B. Villadsen, Jens Abildskov, Philip L. Fosbøl, "BE-Clean: A New P2X desulfurization technology for biogas cleaning", EUBCE 30th, online, 9-12 May 2022 (Poster presentation)

**REGATEC 2022, Malmö, Sweden, 17-18 May, 2022**

Sebastian Borgquist, Sebastian N. B. Villadsen, Jens Abildskov, Philip L. Fosbøl, "A novel desulfurization technology using an electrochemically regenerated oxidant", REGATEC 2022, Malmö, Sweden, 17-18 May 2022 (Poster presentation)

## JUNE

**EAGE Annual General Meeting, Madrid, Spain, 6-9 June 2022**

Einar M. Storebø, Dirk Muter, Ida. L. Fabricius, "Pyrite as an Electrical Conductor in Chalk", EAGE Annual General Meeting, Madrid, Spain, 6-9 June 2022 (Oral presentation)

**SPE Europec, Madrid, Spain, 6-9 June 2022**

Seyedamir Mirazimi, Dan Olsen, Erling H. Stenby, Wei Yan, "Immiscible and Near-Miscible Gas Flooding in Tight Chalk: Laboratory Experiments and Compositional Simulation", SPE Europec, Madrid, Spain, 6-9 June 2022 (Oral presentation)

The 22nd International Conference on Petroleum Phase Behavior and Fouling, PETROPHASE 2022, Bucaramanga, Colombia, 12-16 June 2022

Julia Trancoso, Daniel Qvistgaard, Georgios M. Kontogeorgis, Nicolas von Solms, Even Solbraa, "Vapor-Liquid Equilibrium Measurements and Cubic Plus Association (CPA) Modeling of Triethylene Glycol (1) + Methane/ Ethane (2) + Water (3) Systems", The 22nd International Conference on Petroleum Phase Behavior and Fouling, PETROPHASE 2022, Bucaramanga, Colombia, 12-16 June 2022 (Oral presentation)

**European Conference on Gas Hydrate (ECGH 2022), Lyon, France, 13-16 June, 2022**

Qian Ouyang, Jyoti Shanker Pandey, Yao Xu, Nicolas von Solms, "Characteristics and morphology of CH4/CO2/N2 mixed hydrates using multistep depressurization after hydrate swapping", European Conference on Gas Hydrate (ECGH 2022), Lyon, France, 13-16 June, 2022 (Poster presentation)

**6th International Workshop on Rock Physics, A Coruña, Spain, 13-17 June 2022**

Ermis Proestakis, Leonardo T. P. Meireles, Tobias Orlander, "Reducing uncertainty in shear wave picking of highly porous chalk", 6th International Workshop on Rock Physics, A Coruña, Spain, 13-17 June 2022 (Oral presentation)

Leonardo T. P. Meireles, Ida L. Fabricius, "Strain modeling in a marly chalk reservoir", 6th International Workshop on Rock Physics, A Coruña, Spain, 13-17 June 2022 (Oral presentation)

Leonardo T. P. Meireles, Ida L. Fabricius, "Deriving mineral moduli of the non-carbonate fraction in a marly chalk reservoir using petrophysical logging data and the Isoframe model", 6th International Workshop on Rock Physics, A Coruña, Spain, 13-17 June 2022 (Oral presentation)

Tobias Orlander, Ermis Proestakis, Amirhossein Shamsolhodaei, Helle F. Christensen, "Influence of temperature on dynamic stiffness properties of high porosity North Sea chalk and the governing mechanism", 6th International Workshop on Rock Physics, A Coruña, Spain, 13-16 June 2022 (Oral presentation)

**9th International Conference on Engineering for Waste and Biomass Valorisation, WasteEng2022, Copenhagen, Denmark, 27-30 June 2022**

Cesar Quintela, Evi Peshkepia, Antonio Grimalt-Alemany, Yvonne Nygård, Lisbeth Olsson, Ioannis V. Skiadas, Hariklia N. Gavala, "A two-stage process for enhanced chain elongation during syngas fermentation", 9th International Conference on Engineering for Waste and Biomass Valorisation, WasteEng2022, Copenhagen, Denmark, 27-30 June 2022 (Oral flash presentation)

Qian Ouyang, Jyoti Shanker Pandey, Nicolas von Solms, "Enhanced CO2 Carbon Sequestration by Stepped Depressurization on CH4/CO2 Mixed Hydrates Combined with CH4 Energy Recovery", 9th International Conference on Engineering for Waste and Biomass Valorisation, WasteEng 2022, Copenhagen, Denmark, 27-30 June, 2022 (Oral presentation)

## JULY

**The 32nd European Symposium on Applied Thermodynamics, ESAT 2022, Graz, Austria, 17-20 July 2022**

Evangelos Tsochantaris, X. Liang, G. M. Kontogeorgis, "Evaluation of associated reference thermodynamic models for water's anomalies", The 32nd European Symposium on Applied Thermodynamics, ESAT 2022, Graz, Austria, 17-20 July 2022 (Poster presentation)

Fernando Medeiros, Erling H. Stenby, Wei Yan, "Saturation Point and Phase Envelope Calculation for Systems with Simultaneous Chemical and Phase Equilibrium", The 32nd European Symposium on Applied Thermodynamics, ESAT 2022, Graz, Austria, 17-20 July 2022 (Oral Presentation)

Fernando Medeiros, Erling H. Stenby, Wei Yan, "RAND-based Chemical and Phase Equilibrium Computation: From Standalone Calculation to Dynamic Simulation", The 32nd European Symposium on Applied Thermodynamics, ESAT 2022, Graz, Austria, 17-20 July 2022 (Poster Presentation)

Fufang Yang, T.D. Ngo, Georgios M. Kontogeorgis, Jean-Charles de Hemptinne, "A benchmark database for mixed-solvent electrolyte solutions: Consistency analysis using E-NRTL and example uses in model parameterization", The 32nd European Symposium on Applied Thermodynamics, ESAT 2022, Graz, Austria, 17-20 July 2022 (Oral presentation)

Gabriel M. Silva, Xiaodong Liang, Georgios M. Kontogeorgis, "The limits of the Debye-Hückel models concerning the Poisson-Boltzmann equation", The 32nd European Symposium on Applied Thermodynamics, ESAT 2022, Graz, Austria, 17-20 July 2022 (Oral Presentation)

Gabriel M. Silva, Xiaodong Liang, Georgios M. Kontogeorgis, "The specificities of the different derivations of the Debye-Hückel Equations", The 32nd European Symposium on Applied Thermodynamics, ESAT 2022, Graz, Austria, 17-20 July 2022 (Poster Presentation)

Julia Trancoso, Daniel Qvistgaard, Georgios M. Kontogeorgis, Nicolas von Solms, Even Solbraa, "Vapor-Liquid Equilibrium Measurements and Cubic Plus Association (CPA) Modeling of Triethylene Glycol (1) + Methane/Ethane (2) + Water (3) Systems", The 32nd European Symposium on Applied Thermodynamics, ESAT 2022, Graz, Austria, 17-20 July 2022 (Poster presentation)

Nefeli Novak, I. K. Nikolaidis, G. M. Kontogeorgis, M. Castier, I. G. Economou, "Vapor-Liquid and Liquid-Liquid Equilibria in Electrolyte Solutions: Algorithms and Modeling", The 32nd European Symposium on Applied Thermodynamics, ESAT 2022, Graz, Austria, 17-20 July 2022 (Oral Presentation)

Saman Naseri Boroujeni, Bjørn Maribo-Mogensen, Xiaodong Liang, Georgios M. Kontogeorgis, "A predictive analysis of electrical conductivity models for electrolyte solutions", The 32nd European Symposium on Applied Thermodynamics, ESAT 2022, Graz, Austria, 17-20 July 2022 (Poster Presentation)

Saman Naseri Boroujeni, Bjørn Maribo-Mogensen, Xiaodong Liang, Georgios M. Kontogeorgis, "Electrical conductivity of associative electrolyte solutions", The 32nd European Symposium on Applied Thermodynamics, ESAT 2022, Graz, Austria, 17-20 July 2022 (Poster Presentation)

Yibo Yang, Erling H. Stenby, Alexander A. Shapiro, Wei Yan, Daria Grigorash, "Diffusion Coefficients in Systems Related to Reservoir Fluids:Available Data and Evaluation of Correlations", The 32nd European Symposium on Applied Thermodynamics, ESAT 2022, Graz, Austria, 17-20 July 2022 (Poster presentation)

## AUGUST

**14th International Conference on Applied Energy, ICAE2022, Bochum, Germany, 8-11 August 2022**

Qian Ouyang, Jyoti Shanker Pandey, Yao Xu, Nicolas von Solms, "Enhanced CH4 production and CO2 storage through CH4/CO2/N2 hydrate dissociation during multistep depressurization", 14th International Conference on Applied Energy, ICAE2022, Bochum, Germany, 8-11 August, 2022 (Oral video presentation)

## SEPTEMBER

**The 27th Thermodynamics Conference, Bath, United Kingdom, 7-9 September 2022**

Aswin V. Muthachikavil, Baoliang Peng, Xiaodong Liang and Georgios M. Kontogeorgis, "Hydrogen bonded configurations in liquid water and their correlation with local tetrahedral structures". The 27th Thermodynamics Conference, Bath, United Kingdom, 7-9 September 2022 (Short Oral presentation)

Aswin V. Muthachikavil, Baoliang Peng, Xiaodong Liang and Georgios M. Kontogeorgis, "Hydrogen bonded configurations in liquid water and their correlation with local tetrahedral structures". The 27th Thermodynamics Conference, Bath, United Kingdom, 7-9 September 2022 (Poster presentation)

Evangelos Tsochantaris, Xiaodong Liang, Georgios M. Kontogeorgis, "Using thermodynamic models to describe water's anomalous behavior - Successes and Challenges", The 27th Thermodynamics Conference, Bath, United Kingdom, 7-9 September 2022 (Oral presentation)

Evangelos Tsochantaris, Xiaodong Liang, Georgios M. Kontogeorgis, "Performance of thermodynamic models for water's thermodynamic and structural properties", The 27th Thermodynamics Conference, Bath, United Kingdom, 7-9 September 2022 (poster presentation)

Fufang Yang, T.D. Ngo, J.S. Roa Pinto, Georgios M. Kontogeorgis, Jean-Charles de Hemptinne, "Modeling thermodynamic properties of mixed-solvent electrolyte solutions using ePPC-SAFT". The 27th Thermodynamics Conference, Bath, United Kingdom, 7-9 September 2022 (Poster presentation)

Georgios M. Kontogeorgis, "Thermodynamic modeling of electrolyte solutions". The 27th Thermodynamics Conference, Bath, United Kingdom, 7-9 September 2022 (Poster presentation)

Nefeli Novak, Georgios M. Kontogeorgis, M. Castier, I. G. Economou, "Extension of eSAFT-VR Mie EoS to non-aqueous electrolyte solutions", The 27th Thermodynamics Conference, Bath, United Kingdom, 7-9 September 2022 (Poster Presentation)

Rasmus Fromsejer, Bjørn Maribo-Mogensen, Georgios M. Kontogeorgis, Xiaodong Liang, "Predicting thermodynamic formation properties of solids", The 27th Thermodynamics Conference, Bath, United Kingdom, 7-9 September 2022 (Poster presentation)

Saman Naseri Boroujeni, Bjørn Maribo-Mogensen, Xiaodong Liang, Georgios M. Kontogeorgis, "Thermodynamic properties of associative electrolyte solutions; an implicit solvent model", The 27th Thermodynamics Conference, Bath, United Kingdom, 7-9 September 2022 (Poster presentation).

Saman Naseri Boroujeni, Bjørn Maribo-Mogensen, Xiaodong Liang, Georgios M. Kontogeorgis, "A predictive analysis of implicit solvent models for associative electrolyte solutions", The 27th Thermodynamics Conference, Bath, United Kingdom, 7-9 September 2022 (Poster presentation).

**The 12th International Conference on Distillation & Absorption 2022, Toulouse, France, 18-21 September 2022**

Sebastian Borgquist, Sebastian N. B. Villadsen, Jens Abildskov, Philip L. Fosbøl, "A P2X biogas desulphurization process using an oxidative scrubber", The 12th International Conference on Distillation & Absorption 2022, Toulouse, France, 18-21 September 2022 (Poster presentation)

IWA World Water Congress & Exhibition (IWA), Copenhagen, Denmark 11-15 August 2022

Michael Bache, "Molecular two phase properties of water, can this be exploited?", IWA World Water Congress & Exhibition (IWA), Copenhagen, Denmark 11-15 August 2022 (Oral presentation)

## OCTOBER

**Water Conference 2022 on the Physics, Chemistry and Biology of Water, Bad Söden, Germany, 13-16 October 2022**

Michael Bache, "Study of electromagnetic communication between a chiral drug molecule and its receptor in water", Water Conference 2022 on the Physics, Chemisty and Biology of Water, Bad Söden, Germany, 13-16 October 2022

**GHGT-16, Lyon, France, 23-27 October 2022**

Fernando de A. Medeiros, Duncan Paterson, Erling H. Stenby, Wei Yan, "Novel Geochemical Calculation for Underground Geological Storage of CO2: From Multiphase Geochemical Equilibrium to Compositional Reservoir Simulation", GHGT-16, Lyon, France, 23-27 October 2022 (Oral presentation)

Gcinisizwe Dlamini, Eryk Remiezowicz, Kenneth Ness, Svein-Erik Losnegård, Philip Loldrup Fosbøl, Wentao Gong, Nicolas von Solms, "Optimisation of carbon dioxide conditioning pathways for pipeline sea transport", GHGT-16, Lyon, France, 23-27 October 2022 (Poster presentation)

Isaac Appelquist Løge, Peter Winkel Rasmussen, Randi Neerup, Philip Loldrup Fosbøl, "In-situ measurements of mineral precipitation by means of CT-Scanning", GHGT-16, Lyon, France, 23-27 October 2022 (Poster presentation)

Jens Kristian Jørsboe, Sai Hema Bhavya Vinjarapu, Andreas Christian Møller, Randi Neerup, Søren Jensen, Jakob Lindkvist Karlsson, Philip Fosbøl "Pilot study of CO2 capture for biogas upgrading: Optimization of solvent and process configurations", GHGT-16, Lyon, France, 23-27 October 2022 (poster presentation)

Jens Kristian Jørsboe, Sai Hema Bhavya Vinjarapu, Randi Neerup, Anders Hellerup Larsen, Isaac Appelquist Løge, Andreas Christian Møller, Philip Fosbøl "Monitoring and mitigation of foaming in amine-based CO2 capture processes", GHGT-16, Lyon, France, 23-27 October 2022 (poster presentation)

Randi Neerup, Vasiliki Gkiritzioni, Sai H. B. Vinjarapu, Anders H. Larsen, Valdemar E. Rasmussen, Christina Andersen, Lars K. Gram, Karsten Fuglsang, Jonas Nedenskov, Jannik Kappel, Jens K. Jørsboe, Søren Jensen, Jakob L. Karlsson, Peter Blinksbjerg, Henrik Lassen, Sebastian N. B. Villadsen, Philip L. Fosbøl, "Emission measurements and degradation of solvent from waste incineration plant Amager Resource Centre (ARC), CO2 capture pilot campaign", GHGT-16, Lyon, France, 23-27 October 2022 (Poster presentation)

Randi Neerup, Irene G. Stampino, Isaac A. Løge, Sebastian N. B. Villadsen, Kaj Thomsen, Rolf W. Berg, Philip L. Fosbøl, "Investigation of solid formation in amino acid systems", GHGT-16, Lyon, France, 23-27 October 2022 (Poster presentation)

Sebastian Borgquist, Sebastian N. B. Villadsen, Jens Abildskov, Philip L. Fosbøl, "A P2X biogas desulphurization process using an oxidative scrubber", GHGT-16, Lyon, France, 23-27 October 2022 (Poster presentation)

Seyedamir Mirazimi, Duncan Paterson, Diego Sandoval, Teresa Regueira, Yiqun Liu, Prinu Narayanan, Dan Olsen, Erling H. Stenby, Wei Yan, "Comparison of CO2 and Hydrocarbon Gas Injection in a Low-permeable Chalk Reservoir", GHGT-16, Lyon, France, 23-27 October 2022 (Oral presentation)

Sai Hema Bhavya Vinjarapu, Anders H. Larsen, Randi Neerup, Isaac A. Løge, Valdemar E. Rasmussen, Jens K. Jørsboe, Jakob L. Karlsson, Søren Jensen, Peter Blinksbjerb, Henrik Lassen, Jannik Kappel, Sebastian N. B. Villadsen, Philip L. Fosbøl, "Carbon Capture at Amager Ressourcenter (ARC) Denmark: Challenges and Experiences", GHGT-16, Lyon, France, 23-27 October 2022 (Poster presentation)

Uffe Ditlev Bihlet , Sara Vallejo Castano , Nikolai Andrianov , Sebastian Nis Bay Villadsen , Dirk Koppert , Robert de Kler , Michele Tedesco , Pim Frederix , Philip Loldrup Fosbøl, "The ConsenCUS Project: Carbon Neutral clusters by Electricity-based Innovations in Capture, Utilisation and Storage", GHGT-16, Lyon, France, 23-27 October 2022 (Oral presentation).

**XII Iberoamerican Conference on Phase Equilibria and Fluid Properties for Process Design, EQUIFASE 2022, Campinas, Brazil, 24-27 October 2022**

Gabriel M. Silva, Xiaodong Liang, Georgios M. Kontogeorgis, "The derivations and specificities of the Debye-Hückel equations", XII Iberoamerican Conference on Phase Equilibria and Fluid Properties for Process Design, EQUIFASE 2022, Campinas, Brazil, 24-27 October 2022 (Oral Presentation)

Gabriel M. Silva, Xiaodong Liang, Georgios M. Kontogeorgis, "Investigating the limits of the Debye-Hückel equations concerning the Poisson-Boltzmann equation", XII Iberoamerican Conference on Phase Equilibria and Fluid Properties for Process Design (EQUIFASE 2022), Campinas, Brazil, 24-27 October 2022 (Poster Presentation)

## NOVEMBER

**AIChE 2022 Online, 13-18 November 2022,**

Isaac Appelquist Løge, Peter Winkel Rasmussen , Henning Sørensen Osholm, Anders Nymark, Christensen, Anders Dahl, Benaiah Anabaraonye, Philip Loldrup Fosbøl, Insight to crystallization fouling from 4D X-ray CT: A three step process?", AIChE 2022 Online, 13-18 November 2022 (Poster presentation)

Isaac Appelquist Løge, Benaiah Anabaraonye, Philip Loldrup Fosbøl, "The saturation dependence of BaSO4 surface precipitation kinetics", AIChE 2022, 13-18 November online (Poster presentation)

**LOF, Niels Bohr Institute, Copenhagen, Denmark, 16 November 2022**

Michael Bache, "Hvilke roller spiller vandet for livsprocesserne?", LOF, Niels Bohr Institute, Copenhagen, Denmark, 16 November 2022 (Oral presentation)

**IEA EOR TCP Workshop & Symposium 2022, Stavanger, Norway, 21-24 November 2022**

Fernando de A. Medeiros, Duncan Paterson, Erling H. Stenby, Wei Yan, "A novel framework for geochemical equilibrium calculation in CO2 storage simulation", IEA EOR TCP Workshop & Symposium 2022, Stavanger, Norway, 21-24 November 2022 (Oral presentation)
Seyedamir Mirazimi, Duncan Paterson, Diego Sandoval, Teresa Regueira, Yiqun Liu, Prinu Narayanan, Dan Olsen, Erling H. Stenby, Wei Yan, "Gas injection in a low-permeable chalk reservoir: Comparison between hydrocarbon gas, flue gas, and CO2", IEA EOR TCP Workshop & Symposium 2022, Stavanger, Norway, 21-24 November 2022 (Oral presentation)

**IDA Seminar and Webinar, Havet som energiressource - Havet dækker over 70% af jordens overflade, men udnytter vi havet på den rigtige måde? 28 November 2022, Copenhagen, Denmark**

Michael Bache, "Water molecular research", IDA Seminar and Webinar, Havet som energiressource - Havet dækker over 70% af jordens overflade, men udnytter vi havet på den rigtige måde? 28 November 2022, Copenhagen, Denmark (Oral presentation)

Michael Bache, "Desalination of seawater", IDA Seminar and Webinar, Havet som energiressource - Havet dækker over 70% af jordens overflade, men udnytter vi havet på den rigtige måde? 28 November 2022, Copenhagen, Denmark (Oral presentation)

## DECEMBER

**AGU 2022 Online, 12-16 December 2022**

Isaac Appelquist Løge, Benaiah Anabaraonye, Philip Loldrup Fosbøl, "Surface Investigation of Scale Inhibitors (SISI)", AGU 2022 Online, 12-16 December 2022 (Poster presentation)

Isaac Appelquist Løge, Benaiah Anabaraonye, Philip Loldrup Fosbøl, "The sticking factor: A guide to crystal morphology?", AGU 2022 Online, 12-16 December 2022 (Poster presentation)

# CERE Publications

# CERE Publications, published in 2022

**"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)

**"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)

**"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)

**"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)

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

**"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, (2022) 106568)

**"Importance of the relative static permittivity in electrolyte SAFT-VR Mie equations of state"**
*Pierre J. Walkera, Xiaodong Liangb, Georgios M. Kontogeorgis*
(Fluid Phase Equilibria, 551 (2022) 113256)

**"New insights into the dissociation of mixed CH4/CO2 hydrates for CH4 production and CO2 storage"**
*Jyoti Shanker Pandey, Qian Ouyang, and Nicolas von Solms*
(Chemical Engineering Journal, 427 (2022) 131915)

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

**"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)

**"Novel pore-scale visualization during CO2 injection into CH4 hydrate-saturated porous media"**
*Jyoti Shanker Pandey, Ørjan Strand, Nicolas von Solms, Stian Almenningen and Geir Ersland*
(Energy and Fuels, 36(18) 10552-10571)

**"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 (2022) 54)

**"Comparison of models for the prediction of electrical conductivity of electrolyte solutions"**
*Saman Naseri Boroujeni, Xiaodong Liang, Bjørn Maribo-Mogensen, and Georgios M. Kontogeorgis*
(Ind. Eng. Chem. Res., 61 (2022) 3168-3185)

**"Conclusions from Round Table Discussion 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)

**"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*
(Chemical Thermodynamics and Thermal Analysis, 6 (2022) 100053)

**"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)

**"On the derivations of the Debye-Hückel equations"**
*Gabriel M. Silva, Xiaodong Liang, and Georgios M. Kontogeorgis*
(Molecular Physics, 120 (2022) e2064353)

**"Rigorous phase equilibrium calculation methods for strong electrolyte solutions: The isothermal flash"**
*Ilias K. Nikolaidas, Nefeli Novak, Georgios M. Kontogeorgis, and Ioannis G. Economou*
(Fluid Phase Equilibria, 558 (2002) 113441)

**"A benchmark database for mixed-solvent electrolyte solutions: Consistency analysis using E-NRTL**
*Fufang Yang, Tri-Dat Ngo, Georgios M. Kontogeorgios, Jean-Charles de Hemptinne*
(Ind. Eng. Chem. Res., 61 (2022) 15576-15593)

**"Hydrogen-rich natural gas hydrates formation kinetics in the presence of promoters"**
*Jyoti Shanker Pandey, Jesper Lundtoft Hansen, Nicolas von Solms*
(Chemical Engineering Journal, 432 (2022) 134295-)

**"Investigation of the limits of the linearized Poisson-Boltzmann equation"**
*Gabriel M. Silva, Xiaodong Liang, Georgios M. Kontogeorgis*
(J. Phys. Chem. B, 126 (2022) 4112–4131)



**"Stiffness control in dual color tomographic volumetric 3D printing"**
*Bin Wang, Einstorm Engay, Peter R. Stubbe, Saeed Z. Moghaddam, Esben Thormann, Kristoffer Almdal, Aminul Islam, Yi Yang*
(Nature Communications, 13 (2022) 367)

**"Design and analysis of novel CO2 conditioning process in ship-based CCS"**
*Wentao Gong, Eryk Remiezowicz, Philip Loldrup Fosbøl, Nicolas von Solms*
(Energies, 15 (2022) 5928) (Presented at the 15th International Conference on Greenhouse Gas Control Technologies, GHGT-15, Abu Dhabi, UAE, March 2021)

**"Critical Parameters Influencing Mixed CH4/CO2 Hydrates Dissociation during Multistep Depressurization"**
*Qian Ouyang, Jyoti Shanker Pandey, Nicolas von Solms*
(Fuel, 320 (2022) 123985)

**"Computer-aided multifunctional ionic liquid design for the electrolyte in LTO rechargeable batteries"**
*Yingjun Cai, Yuqiu Chen, Haitao Zhang, Nicolas von Solms, Georgios Kontogeorgis, John M. Woodley, Kaj Thomsen*
(J. Phys. Chem. C, 126 (2022) 11498-11509)

**"The true Hückel equation for electrolyte solutions and its relation with the Born term"**
*Gabriel M. Silva, Xiaodong Liang, Georgios M. Kontogeorgis*
(Journal of Molecular Liquids, 368 (2022) 120554)

**"Solid-liquid phase boundaries in the system: glycine-NaOH-NaHCO3-H2O"**
*Randi Neerup, Irene G. Stampino, Kaj Thomsen, Rolf W. Berg, Sebastian N. B. Villadsen, Philip L. Fosbøl*
(J. Chem. Eng. Data, 67 (2022) 1550-1564)

**Review of barium sulphate solubility measurements**
*Lucas F.F. Corrêa, Jiasheng Hao, Randi Neerup, Susana Almeida, Meng Shi, Kaj Thomsen, Philip L. Fosbøl*
(Geothermics, 104 (2022) 102465)

**"A new view on scale"**
*Isaac Løge Appelquist, Randi Neerup, Philip Loldrup Fosbøl*
(SPE-209512-MS (2022))

**"A view on the future of applied thermodynamics"**
*Jean-Charles de Hemptinne, Georgios Kontogeorgis, Ralf Dohrn, Ioannis G. Economou, Antoon ten Kate, Susanna Kuitunen, Ljudmila Fele Žilnik, Maria Grazia De Angelis, and Velisa Vesovic*
(I&EC Research, 61 (39) (2022) 14664-14680)

**"Modeling binary and multicomponent systems containing supercritical CO2 with polyethylene glycols and compounds relevant to the biodiesel production"**
*Ioannis Tsivintzelis, George Koutsou, and Georgios M. Kontogeorgis*
(Molecules, 27 (2022) 5785)

**"Synthesis and in situ sulfidation of molybdenum carbide MXene using fluorine-free etchant for electrocatalytic hydrogen evolution reactions"**
*Binesh Unnikrishnan, Chien-Wei Wu, Arumugam Sangili, Ya-Ju Hsu, Yu-Ting Tseng, Jyoti Shanker Pandey, Huan-Tsung Chang, Chih-Ching Huang*
(Journal of Colloid and Interface Science, 628 (2022) 849-857)

**"Insights into multistep depressurization of CH4/CO2 mixed hydrates in unconsolidated sediments"**
*Qian Ouyang, Jyoti Shanker Pandey, Nicolas von Solms*
(Energy, 260 (2022) 125127)

**"Influence of CO2 on the solubility of potassium glycinate in glycine-KOH-H2O, glycine-KHCO3-H2O, and glycine-KOH-KHCO2-H2O"**
*Valdemar E. Rasmussen, Randi Neerup, Irene G. Stampino, Sai H. B. Vinjarapu, Sebastian N. B. Villadsen, Kaj Thomsen, and Philip L. Fosbøl*
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**"Conformational triggering in voltammetry and single-molecule conductivity of two-centre redox metalloproteins: Cytochrome c4 and copper nitrite reductase"**
*Henrik Bohr, Irene Shim, Jens Ulstrup, Xinxin Xiao*
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**"Reference density database for 20 aqueous alkali halide solutions"**
*Fufang Yang, Jingang Qu, Georgios M. Kontogeorgis, and Jean-Charles de Hemptinne*
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**"Extended UNIQUAC thermodynamic modeling of aqueous two-phase systems, water + salt + short-chain alcohol"**
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**"Insights into multistep depressurization of CH4/CO2 mixed hydrates in unconsolidated sediments"**
*Qian Ouyang, Jyoti Shanker Pandey, Nicolas von Solms*
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**"Formation of robust CEI film on high voltage LiNi0.6C00.2Mn0.202 cathode enabled by functional [PIVM] [TFSA] ionic liquid additive"**
*Yingjun Cai, Tinghua Xu, Xianglei Meng, Nicolas von Solms, Haitao Zhang, Kaj Thosen*
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**"Crossover residual entropy scaling of the viscosity and thermal conductivity of carbon dioxide"**
*Hangtao Liu, Fufang Yang, Zhen Yang, Yuanyuan Duan*
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**"Structural characteristics of low-density environments in liquid water"**
*Aswin V. Muthachikavil, Georgios M. Kontogeorgis, Xiaodong Liang, Qun Lei, and Baoliang Peng*
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**"Diffusion coefficients in systems related to reservoir fluids: Available data and evaluation of correlations"**
*Yibo Yang, Erling H. Stenby, Alexander A. Shapiro, and Wei Yan*
(Processes, 10 (2022) 1554-)



**"Impact of gas liberation effects on the performance of low permeability reservoirs"**
*Nikolai Andrianov, Niels Marinus Bech, Carsten Møller Nielsen, Wael Al-Masri, and Alexander Shapiro*
(Energies, 15 (2022) 3707-)

**"Unified thermodynamic modelling of diffusion and thermodiffusion coefficients"**
*Hadise Baghooee, Alexander Shapiro*
(Fluid Phase Equilibria, 558 (2022) 113445-)

**"Continuous upscaling of the 3D diffusion equation in a heterogeneous medium"**
*Alexander A. Shapiro*
(Chemical Engineering Science, 248 (2022) 117247)

**"Befæstet af begroning"**
*Isaac Appelquist Løge, Benaiah U. Anabaraonye, Philip Loldrup Fosbøl*
(Dansk Kemi, 103(5) (2022) 24-26)

**"Synthetic case study: discrimination of unexploded ordnance (UXO) and non-UXO sources with varying remanent magnetization strength using magnetic data"**
*Mark David Wigh, Thomas Mejer Hansen, and Arne Døssing*
(Geophysical Journal International, 228 (2022) 773-791)

**"High-speed magnetic surveying for unexploded ordnance using UAV systems"**
*Mick Emil Kolster, Mark David Wigh, Eduardo Lima Simöes da Silva, Tobias Bjerg Vilhelmsen, and Arne Døssing*
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**"On the implementation of a preconditioned Riccati Recursion based Primal-Dual interior-point algorithm for input constrained optimal contral problems**
*Morten Ryberg Wahlgreen, John Bagterp Jørgensen*
(IFAC PapersOnLine 55-7 (2022) 346-351)

**"Modeling and simulation of upstream and downstream processes for monoclonal antibody production"**
*Morten Ryberg Wahlgreen, Kristian Meyer, Tobias K. S. Ritschel, Allan Peter Ensig-Karup, Krist V. Gernaey, John Bagterp Jørgensen*
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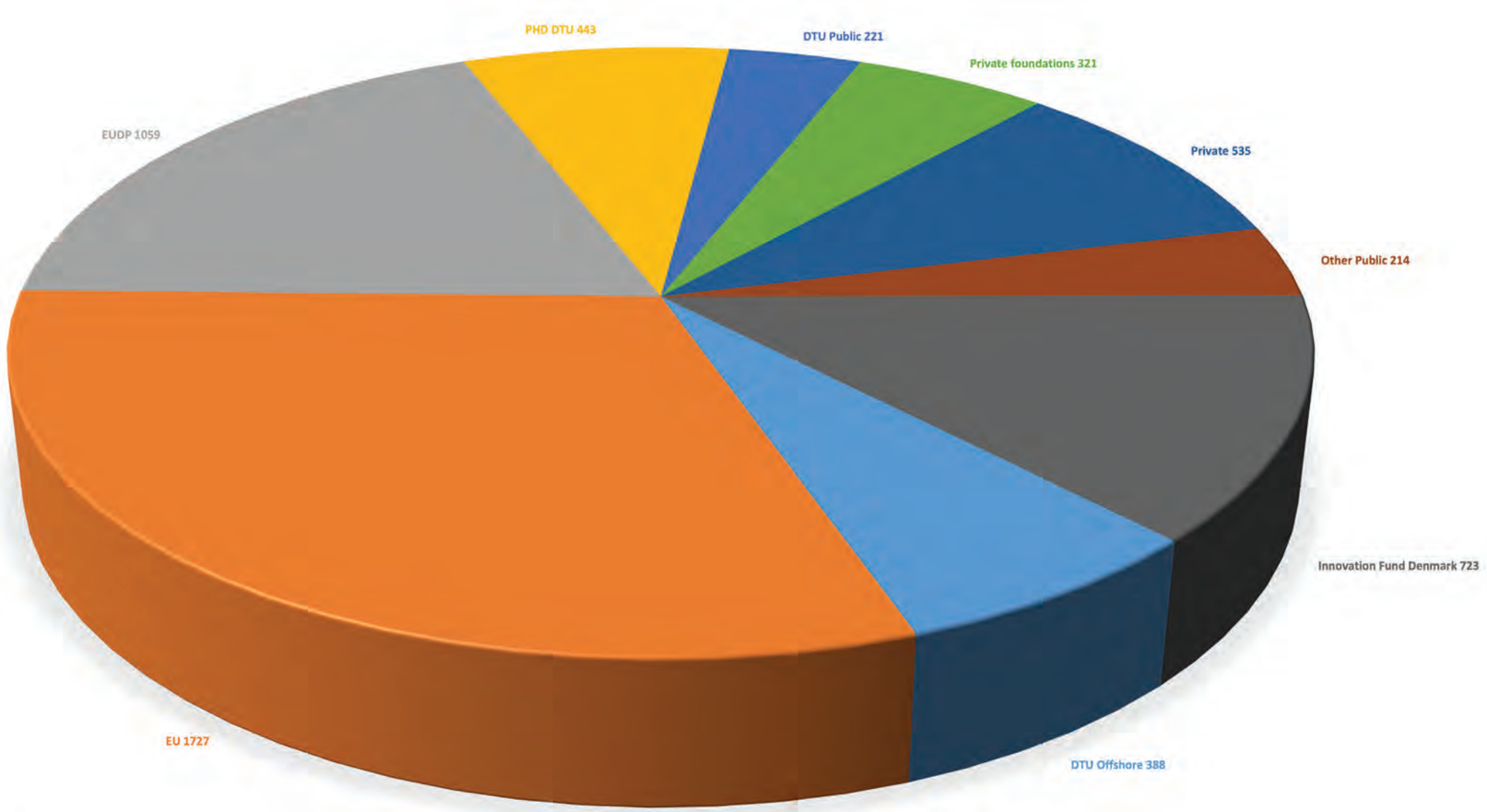


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