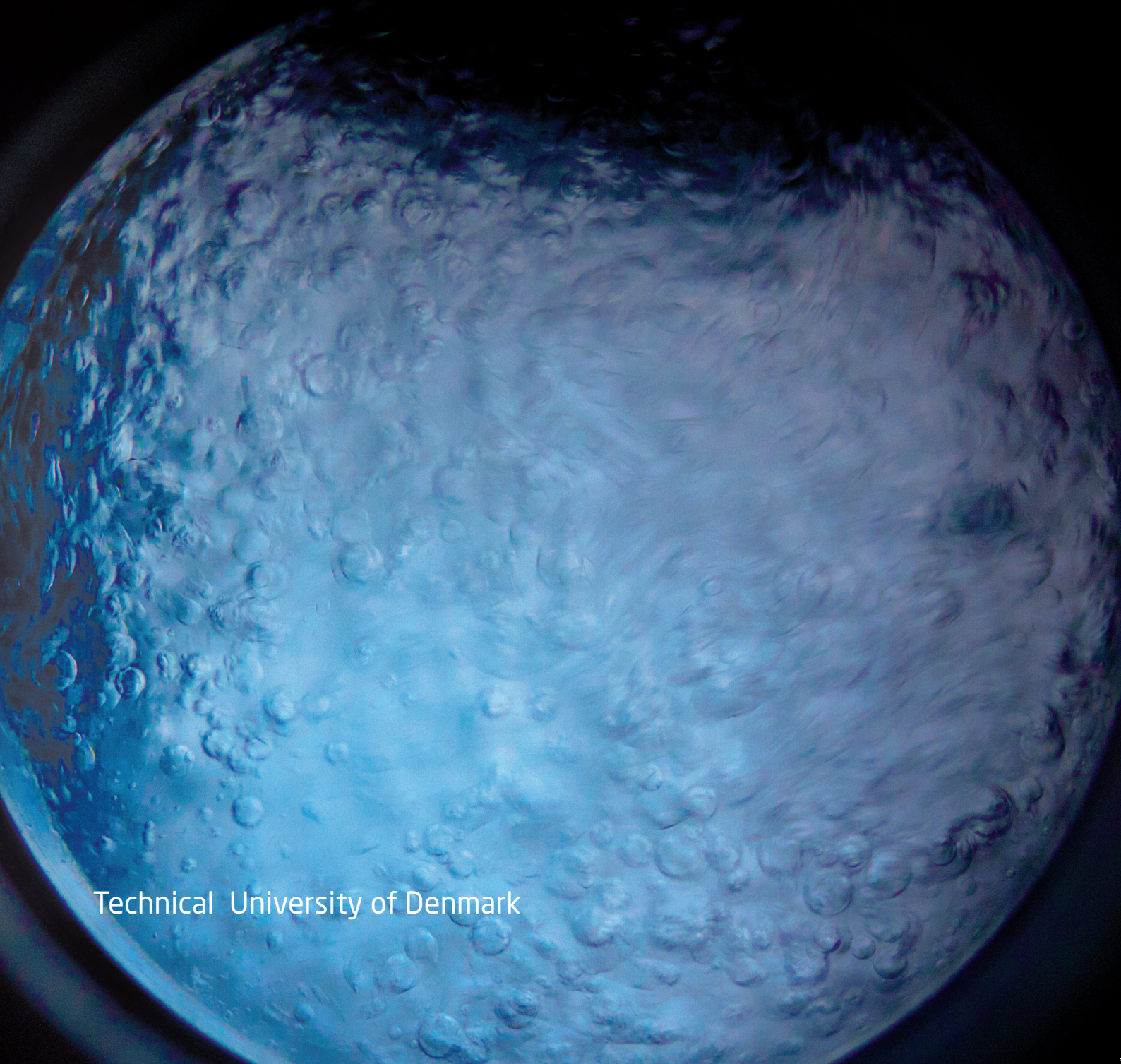
DTU

Annual Report 2010

CERE

Center for Energy Resources Engineering



Technical University of Denmark

CERE Annual Report 2010

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The picture shows the stirring of water and propane at low temperature just prior to the formation of the gas hydrate (i.e., propane hydrate). Propane is present here both as a gas and as small droplets dispersed in the water phase. The picture has been taken through the sapphire windows of a high-pressure stainless steel cell.
Photo: Christian Carlsson, CERE DTU

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CERE's Jump Start

Erling H. Stenby
Director of CERE,
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Already in its first year, Center for Energy Resources Engineering has set a course that justifies our new name and structure.

Structural changes, no matter how carefully planned they may be, will always be followed by a certain level of anxiety. As for the transformation into Center for Energy Resources Engineering from our previous organization we could hardly have wished for a better debut.

A new project within geothermal energy has attracted significant research funding which will raise the understanding of this relatively novel and renewable energy source and its potential in Denmark. The project is headed by geologist, Associate Professor, Dr. Sc. Ida Lykke Fabricius, and will also involve geophysicist, Professor Klaus Mosegaard. Both are new members of the CERE Faculty.

The project on geothermal energy will also involve partners in CERE's industrial Consortium and a number of other CERE Faculty members, mainly working within thermodynamics – making the project truly interdisciplinary. This underlines the potential of the CERE construction.

Chalk breakthrough

Also the centre's traditional core areas have contributed to our jump start.

In August CERE was proud to host a SPE (Society of Petroleum Engineers) workshop symposium where the results of a truly interesting research finding were presented – namely that carbon dioxide flooding seems to be an EOR (Enhanced Oil Recovery) method which is surprisingly efficient when applied to a tight chalk reservoir. These findings attracted considerable attention from our stakeholders, ranging from industry and academia to government, press and research administration. Please find more information on the project on the following pages.

Another finding which attracted broad attention was research by Ph. D. Lars Jensen and Associate Professor Nicolas von Solms into proteins as gas hydrate inhibitors in oil recovery. Also, Nicolas von Solms has just received substantial funding from the Danish Research Council for Independent Research / Technology and Production Sciences for the continuation of the project. With a merely 8 per cent success rate for applications to the council, we see this as yet another confirmation of the high quality work performed at the center.

Just like the findings on EOR in tight chalk, the results on proteins as gas hydrate inhibitors attracted wide press coverage. While media attention should not be a goal in itself to a research center like ours, we are happy to have the opportunity to disseminate our results to a broader audience. Especially as a newly created center this type of positive attention is of high value.

High profile on carbon capture

As already seen by the new geothermal energy project the term Energy Resources Engineering does not refer to oil and gas exclusively. Another high profile area is Carbon Capture and Storage (CCS). At CERE we see ourselves as a part of responsible transition to a sustainable energy future and believe that CCS will be a highly needed element. The center maintains a high level of activity within capture technologies. As CCS moves closer to implementation, the center's resources within geology and geophysics will become increasingly relevant.

Finally I would like to stress that CERE's name in no way implies a lower priority given to those projects at the centre which are not related to energy. Much to the contrary we will also be able to strengthen research related to chemical industry processes, food manufacturing and others. Therefore, please feel free to address any project enquiries to the undersigned or any of the other members of the CERE group – we are always happy to discuss new openings as well as further expansions of already well-known areas.

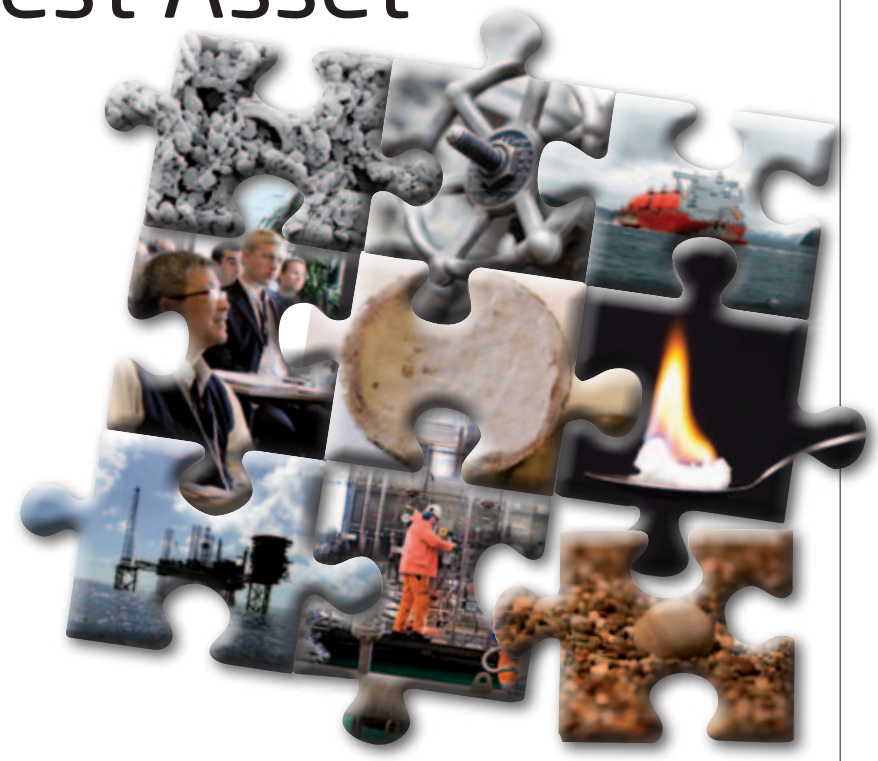
Professor Erling H. Stenby,
Director of CERE

A more detailed summary of 2010 events to be found at page 28

The Consortium – our Strongest Asset

CERE is supported by public means from several sources, e.g. The Danish Council for Independent Research / Technology and Production Sciences and the EU. Furthermore the center is supported by grants from several private companies.

The strongest asset of CERE is the industrial Consortium. Approximately 25-30 companies are members, the exact number changes due to the dynamics of the industry's mergers and acquisitions. The member companies closely follow the activities of the center. This ensures that CERE activities are relevant in relation to the topical problems and limitations in existing knowledge. This on-going external control of quality and inspiration assists in maintaining CERE research at the highest international level.



CERE Consortium:

● Statoil ● Maersk Oil ● GDF-SUEZ ● ConocoPhillips ● Haldor Topsøe ● BP ● Linde ● Eni ● Total ● DONG Energy ● Shell ● GASSCO ● OMV ● Chevron ● Petrobras ● SQM ● RWE ● Akzo Nobel ● IFP ● Schlumberger ● ExxonMobil ● Vattenfall ● Welltec ● Saudi Aramco ● Sinopec ● Lloyd's Register ODS

Brand new projects in CERE

After deadline for this report the center was granted two large projects from the Danish Advanced Technology Foundation. The first project, BioRec - Biotechnology in Oil Recovery - is a unique partnership between oil and biotechnology, respresented by Maersk Oil and DONG Energy, and Novozymes, respectively. CERE will lead the project, and the other project partners are the University of Roskilde and the Danish Institute of Technology. The vision of the project is to develop biotechnological knowledge and technology to increase the amount of recoverable oil in Danish oil fields in the North Sea. This will be achieved by development of biotechnological tools that are significantly more efficient, more economically viable and environmentally safer than existing solutions. The overall budget is EUR 4.5 mio, where the Foundation supports with EUR 2 mio and Industry with EUR 1.5 mio.

The second project is a partnership between CERE-DTU and the Danish sonar company, Reson A/S. This project aims to develop a model for oil-polluted sea water and from there, a state-of-the-art sonar product with an effective method for the detection and quantification of oil in sea water. The overall budget for this project is EUR 2.3 mio., where the Danish Advanced Technology Foundation supports the project with EUR 1.4 mio and Industry further adds EUR 0.5 mio.

A Breakthrough for Recovery in Tight Chalk

According to a recently finalized grand-scale Danish research project with CERE in a central role it seems realistic to raise expectations for the overall recovery rate in the Danish part of the North Sea from 30 to 45 per cent. The optimism is founded on laboratory experiments from carbon dioxide flooding in chalk with low permeability.

Carbon dioxide flooding seems to be an EOR (Enhanced Oil Recovery) method which is surprisingly efficient when applied to tight chalk reservoirs. For instance, roughly half of known oil reserves in the Danish part of the North Sea are found in chalk with extremely low permeability from the so called Danien period. This is one of the main reasons why expectations for the overall recovery rate for the Danish part of the North Sea have so far been kept at 30 per cent or below. New results from this Danish research project on CO_2 EOR indicate that it could be possible to recover as much as 45 per cent.

In laboratory experiments under realistic conditions a 90 per cent recovery rate was achieved using carbon dioxide flooding in Danien chalk.

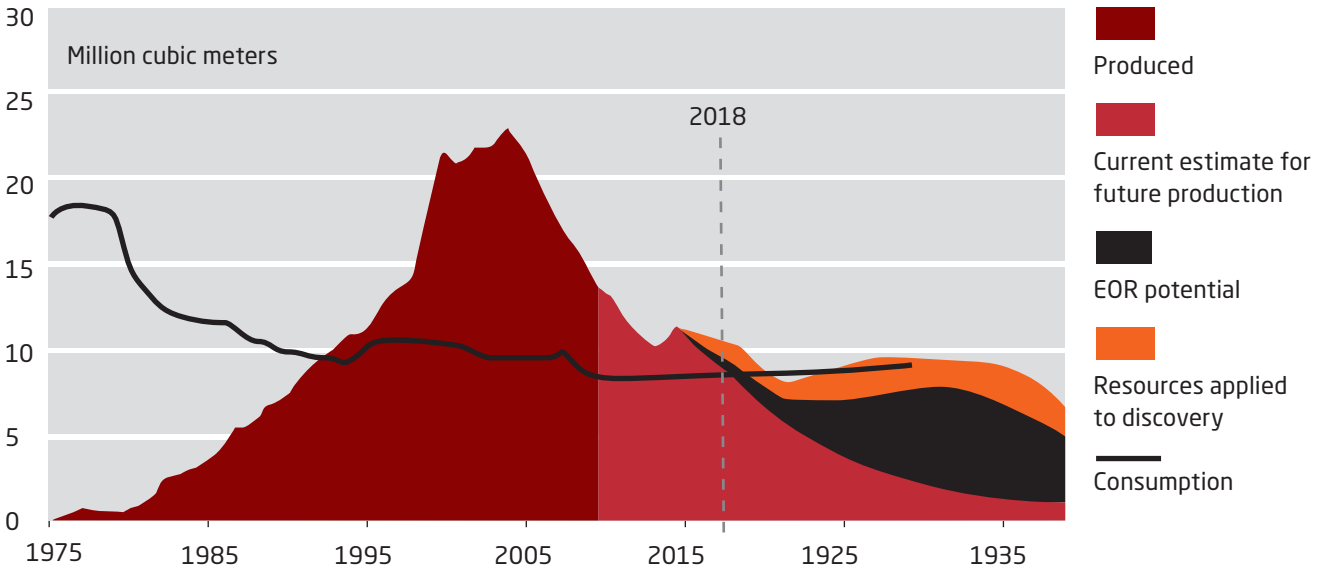
The partners behind the project are CERE, DONG Energy, GEUS (The Geological Survey of Denmark and Greenland) and geological consultants GEO. The project was supported by The Danish National Advanced Technology Foundation (Højteknologifonden).

The project also addressed the risk of reservoir collapse.

"Before this project it was still unclear whether carbon dioxide injection would weaken the chalk, causing risk of reservoir collapse which would be a major drawback. However, interestingly enough, the results from our laboratory experiments have

Production and possible future development

Overall production history and possible future development for oil recovery in the Danish part of the North Sea. The black zone represents the scope for EOR.



Source: The Danish National Energy Board (Energistyrelsen)

In laboratory tests up till 90 per cent of oil contained in tight chalk samples was recovered.

demonstrated that carbon dioxide injection does not imply a higher risk compared to traditional water flooding," comments Professor Erling H. Stenby, Director of CERE, while adding:

"Overall it is hard to see drawbacks to the new technique and we have of course noted considerable interest from industry."

An additional benefit from carbon dioxide flooding EOR is to benefit climate protection. Carbon dioxide is a major contributor to global warming and oil reservoirs are one of the prospective geological structures for carbon dioxide storage. Carbon dioxide storage in oil reservoirs has several advantages, especially for quick implementation. Besides the economic benefit – from recovering more oil – the technology has been developed over more than 30 years reaching a level of maturity. Also, the abundant data concerning geological information of reservoirs have been accumulated.

"Closing the EOR Loop"

Another CERE project also addressing EOR but in a more generic fashion is the ADORE (Advanced Oil Recovery Methods) project sponsored by the Danish Research Council for Technology and Production, DONG Energy and Maersk Oil. This project lays the foundation for several of the more applied projects in CERE. Fredrik Saaf, Reservoir Engineer at Shell, chairman of the Advisory Board for the ADORE project, comments:

"The ADORE project brings a uniquely comprehensive approach to raising our understanding of EOR processes, particularly their application in Danish chalk reservoirs.

A five-pronged research effort under the direction of Professor Erling H. Stenby, ADORE is host to a team of world-class experts tackling problems in the diverse focus areas of Reactive Transport, Phase Behavior, Flow in Porous Media, Rock Mechanics and Numerical Methods, with the common objective of producing research that will ultimately help adding to recoverable hydrocarbon reserves via novel or improved EOR methodologies.

ADORE's research is certainly grounded in sound empirical methods, but it is not mired in

tradition or limited to conventional approaches; indeed, there is a commendable willingness to pursue unconventional, riskier topics as well. Examples range from investigating the success factors for Microbial EOR (MEOR) and In-Situ Combustion (ISC), to challenging and reformulating the established laws of multiphase subsurface flow in pursuit of more accurate engineering models.

The recent inception of the Center for Energy Resources Engineering (CERE) at DTU deserves special mention as it is certain to bring important benefits also to ADORE in the form of natural synergies with other groups within CERE, such as Carbon Capture and Sequestration (CCS). There is a strong potential for the ADORE group of further "closing the loop" on EOR problems, owing to the additional multidisciplinary possibilities that CERE creates."

New results from a Danish research project on CO_2 EOR indicate that it could be possible to recover as much as 45 per cent of oil in the Danish part of the North Sea. Photo: DONG Energy A/S.

PhD Defense

CO_2 Flooding in Chalk Reservoirs

Ben Niu
PhD. Today works at CERE as Post doc
Supervisor:
Alexander Shapiro

A range of techniques have been developed and applied to improve oil recovery to meet the increasing demands on energy resources. A new dawn of CO_2 flooding is coming and it is expected to continue to expand in the near future for two reasons. Firstly, increasing costs related to other methods favour CO_2 flooding – i.e. increasing energy costs drive costs for thermal EOR projects upwards, while the same is true of the price for natural gas that could be used for EOR related injection. Secondly, climate change requires reduction of CO_2 concentration in the atmosphere.

The thesis addresses CO_2 injection in chalk reservoirs by both experimental work and a modelling study.

The experimental work focuses on improving the current methods for determination of in situ phase saturation during CO_2 flooding in low permeable chalk at reservoir conditions. A number of trial CO_2 flooding experiments and two successful tertiary flooding experiments have been completed. A major part of the experimental work is dedicated to use of X-ray CT scanning as an assisting tool in core analysis. Also, new experimental methods have been proposed and applied on North Sea chalk using live oil. Detailed data analysis indicates successful application of the methods proposed.

The modelling study focuses on coupling geochemical reactions with multiphase flow in enhanced oil recovery (EOR) processes. While studies of multiphase flow and thermodynamic properties of CO_2 and oil can be considered a mature field of research, still some basic questions have not been answered yet. One of them is insight into the flow inside the porous media to investigate how different phases flow and how the miscibility develops. Visualization of CO_2 flow in core samples under reservoir conditions is one way to bridge the gap between mathematical models on short-term CO_2 flooding and those on long-term CO_2 storage.

PhD Defense

Microbial Enhanced Oil Recovery – Advanced Reservoir Simulation

Sidsel Marie Nielsen
PhD. Today works at CERE as Post doc
Supervisor:
Alexander Shapiro

In Microbial Enhanced Oil Recovery (MEOR), either bacteria are injected together with nutrients or indigenous bacteria are activated by injection of nutrients. The efficiency of MEOR is related to two main mechanisms; reduction of the interfacial tension (IFT) due to surfactant production, and microscopic fluid diversion as a part of the overall fluid diversion mechanism due to formation of biofilm.

Both mechanisms may lead to an increase in flow rate of oil. The thesis investigates both mechanisms by use of a one-dimensional generic model.

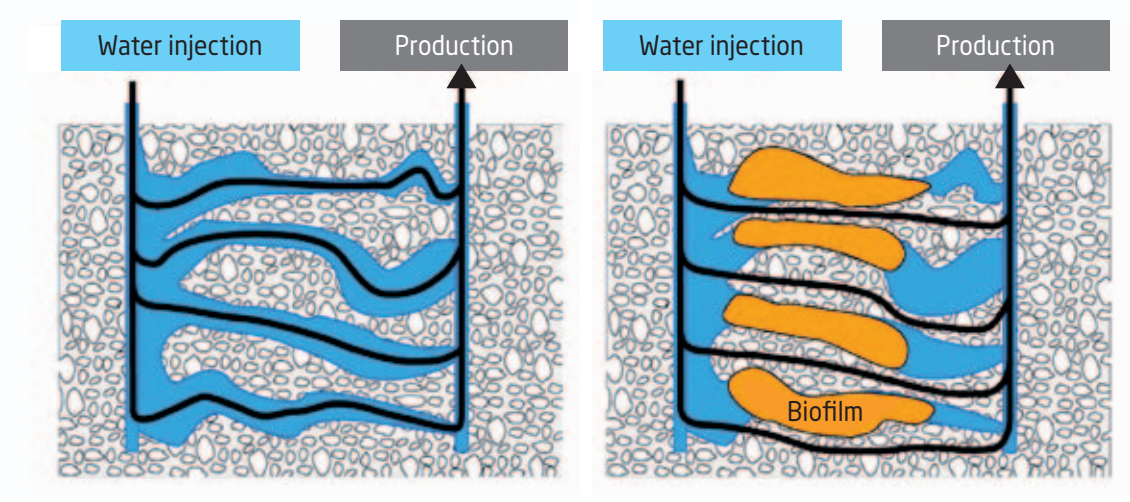
The thesis uses a novel approach in relation to MEOR, the partition of surfactant between oil and water. Surfactant is the key component in order to reduce IFT.

It was found that final recovery depends on how much the surfactant-induced IFT reduction lowers the residual oil, which is also a result of efficiency of the surfactant. A super efficient surfactant produces an incremental recovery around 40 per cent over that of water flooding. Application of a less efficient – and probably more realistic – surfactant results in an incremental oil recovery of 9 per cent above water flooding, which is still considered a significant improvement.

Under the right conditions bacteria will form so called biofilms consisting of a mixture of the bacteria themselves, particles and substances produced by the bacteria serving as a kind of glue. Biofilm formation may increase the MEOR recovery rate further.

The one-dimensional studies for the mechanisms separately and in combination show that all the mechanisms contribute to improvement of oil recovery. The mechanisms produce their characteristic effect on the saturation profile and thus on the recovery curve. When sufficient amounts of surfactant can be produced, the effect from surfactant generates a larger effect compared to microscopic fluid diversion.

In the study an improvement in recovery rate against water flooding of 15 per cent was achieved under realistic conditions by a combination of biofilm formation, microscopic fluid diversion and surfactant production.



The principle of Microbial Enhanced Oil Recovery (MEOR). In the study an improvement in recovery rate against water flooding of 15 per cent was achieved under realistic conditions by a combination of biofilm formation, microscopic fluid diversion and surfactant production.

Energy Savings beneath Our Feet

Heat is plentiful during summer. Using the right geological structures for intermediate storage we can transfer our natural summertime energy surplus till wintertime where it is more needed. The technology is in principle well established, costs would be small and as carbon dioxide emissions will be negligible, the method would contribute to climate protection. Benefits could be even larger if combined with geothermal energy and district heating.

No imports of raw materials are required to put this climate friendly idea into practise, neither do we have to await development of new, innovative technology. Conditions are already at hand – or rather, they are present beneath our feet! Especially during summertime, our energy system has a relative surplus of heat. This surplus can be stored in geological structures till winter.

"Heat storage will undoubtedly become a key issue in the future. Whether you would ask the government, the opposition or the national climate commission they all emphasize the need to become independent of fossil fuels. If we are to achieve just that, heat storage will be a part of the solution since, as we turn to more renewable energy, fluctuations in production will be larger," says Jesper Magtengaard, Senior Asset Manager for Geothermal Energy at DONG Energy, adding:

"The best solution in my view would be to combine seasonal heat storage with geothermal energy exploitation. The installations should be relatively large with wells into deep, warm aquifers. This will minimize heat loss. Each installation would consist of at least four wells; two for geothermal production and two for water injection. In summertime where the demand for heat is small, the water from one of the two production lines could be heated by surplus heat and injected back into the aquifer."

"We see this as short cut to large storage capacity. Costs will be modest. If you take a look at the technology required, it is all pretty much available. We already have experience in drillings involving pumps able to tolerate water at up till 180 degrees C. Further developments are expected to allow temperatures up till 200 or even 220 degrees C."

Choose a warm aquifer

The surplus heat to be stored in summertime could be solar energy, waste incinerated heat or electricity at low prices.

"As fall comes your heat storage aquifer will be very warm. This heat can be tapped during fall and winter in situations of peak demand – saving fossil fuels and lowering carbon dioxide emissions," says Jesper Magtengaard.

When calculating the climate effect of the concept one should of course subtract energy consumption related to running the system; this would mainly be power for the pumps that drive water injection and extraction. However, if designed wisely this consumption – and associated carbon dioxide emission – will be tiny compared to the amounts of emissions avoided by the heating energy gained.

"I believe this idea should be put to use on a larger scale and at least the potential scope should be investigated," agrees geologist Ida Lykke Fabricius, Dr. Sc. and Associate Professor at CERE. She is also a member of the DTU Environment faculty.

Storing heat from summer till winter is often referred to as ATES – Aquifer Thermal Energy Storage. However, Ida Lykke Fabricius advocates a modified version of the concept:

"The term ATES is often connected with storing heated water in a random aquifer, which would often be a relatively cold aquifer. Why not choose a warm aquifer? This would lower the heat gradient, minimizing the loss of heat to the surroundings. Ideally we would combine ATES with geothermal energy. This would harvest the

"If you look at the thoughts of the national climate commission and general trends in energy policy, my guess is that heat storage capacity will be acutely in demand somewhere around 2025. This doesn't allow much time for hesitation. The research should be initiated as soon as possible."

Jesper Magtengaard, Senior Asset Manager, Geothermal Energy, DONG Energy

full benefit of the infrastructure established."

The concept would be especially interesting to a country like Denmark where district heating is already advanced, she emphasises:

"One could use the geothermal and stored heat directly for district heating. Further the source for storing heat during summertime might not only be water heated by the Sun as traditionally in ATES. A number of countries – Denmark being one of them – are about to engage in bio fuels also for heating. It might be economically rational to let these plants run throughout the year and let the heat produced in summertime be stored for later use. The same thing applies to incineration of waste which is also used for heating purposes i.e. in Denmark. The systems requires for the waste to be burned throughout the year. Presently part of the heat is just being wasted in summertime. It should be utilized."

Scientific homework comes first

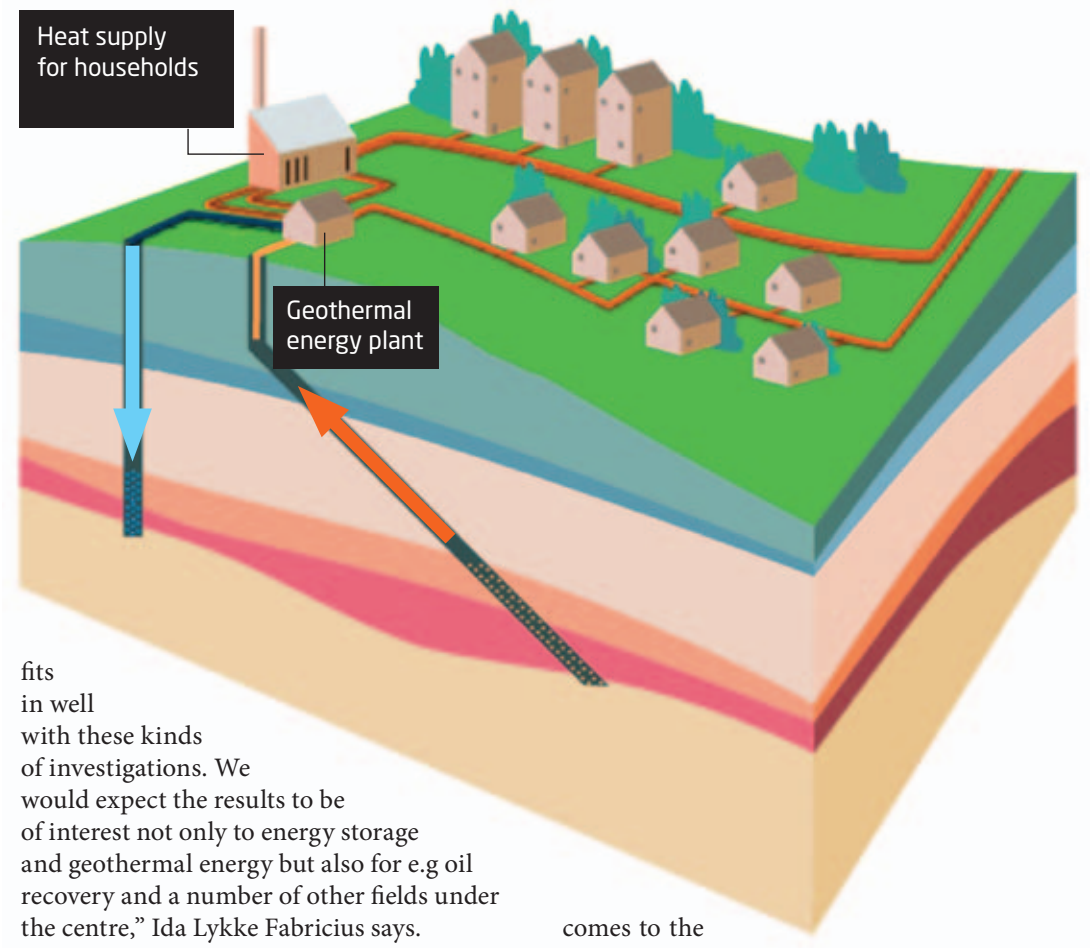
A further attraction is the fact that the idea does not require new technology to be developed. ATES is already running on a small scale – i.e. there are some 20-30 installations supplying individual buildings in Denmark – and the technology for injecting water into aquifers and later extracting it is well proven. Still, if the concept is to be lifted from individual buildings to cities or even a regional or national scale there is initial research and development to do.

"Firstly, surveys should establish the structures with the largest potential for storing heat. These findings should be compared with the geography of consumption to find the locations of most interest. Secondly, there are a number of geophysical and thermodynamic questions that would need to be answered. This is where the main interest of CERE comes in," Ida Lykke Fabricius explains.

The questions relate to how the additional heat added to the geological structures will affect them. What will happen to their stability and permeability? And which methodology should be applied for keeping track of these developments?

"The expertise here at CERE in both modelling and simulation and in experimental work

Geothermal action. Before establishing a geothermal production facility, local geology is mapped by seismic measurements. The image is from 2007 when seismic measurements were undertaken in a joint project by district heating company Sønderborg Fjernvarme and DONG Energy.
Photo: Dong Energy A/S



Principle drawing for geothermal production – the geothermal pilot plant at Margretheholm, Denmark.

fits in well with these kinds of investigations. We would expect the results to be of interest not only to energy storage and geothermal energy but also for e.g oil recovery and a number of other fields under the centre," Ida Lykke Fabricius says.

> Firstly, surveys should establish the structures with the largest potential for storing heat. These findings should be compared with the geography of consumption to find the locations of most interest
>
> **Ida Lykke Fabricius, Associate Professor, CERE**

Now is the time to start

Jesper Magtengaard of DONG Energy is supportive:

"Uncertainty about what injection of hot water will do to the aquifer remains a barrier to the individual district heating plants considering whether to engage in the technology. Will the extra heat lead to chemical precipitation of various substances? This is an important question to answer and it lies beyond the single plant to address – a national effort is required."

"This is why CERE's new initiative is extremely relevant. Until this uncertainty is resolved we can not expect the district heating sector to invest. At DONG Energy we are backing the initiative and we are ready to contribute with cases to ensure that calculations are based on realistic scenarios. Further, we are offering our know-how when it comes to the necessary linking of the heat storage and geothermal energy exploitation to the existing energy infrastructure. I am also aware that a number of district heating companies are ready to participate. This will further secure the relevance of the project."

"A research program of this scope requires four years to resolve the issues in question. If you look at the thoughts of the national climate commission and general trends in energy policy, my guess is that heat storage capacity will be acutely in demand somewhere around 2025. This doesn't allow much time for hesitation. The research should be initiated as soon as possible."

The Danish Council for Strategic Research has approved a budget of close to 2.0 million EUR for a Danish research program on geothermal energy led by CERE.

High Schools Engage in Oil Discovery

More than one thousand Danish high school students took part in the 2010 version of the PetroChallenge competition.

Since its introduction in 2005, the Danish version of the international PetroChallenge competition has steadily attracted a growing number of high schools, setting a new record for participation each year. 1,100 students from 30 high schools engaged in the competition's virtual hunt for undiscovered offshore oil reserves in 2010.

"The students learn about oil and a number of disciplines within the natural sciences and even social sciences – i.e. they are required to choose from a range of possible investment strategies and engage in partnerships with other players. Further, a fair part of communication is done in English. But still an even larger attraction is, in my view, that they improve their ability to work in a group. They are required to make a number of key decisions as they go along and they will only be able to perform well if they cooperate," says cand. scient. Tove Holm Petersen, Svendborg Tekniske Gymnasium.

For several high schools participation has become an annual tradition. One of them is the technical high school (HTX) in Svendborg where all first year students participate – meaning more than one hundred students.

"We gather everybody in the same hall and set up screens where you can follow the current standings. The two days of competition are lots of fun. Many second and third year students drop by just to see if the freshmen are representing our high school well. Towards the final moments things get quite wild and competitive. It is a matter of honour!" Tove Holm Petersen explains.

The Danish branch of the PetroChallenge competition is organized by CERE. In all countries involved, students use the OilSim simulation tool developed by Simprentis – a tool also applied in real oil discovery.

During the competition the various phases of oil discovery are simulated. Including one realistic feature - with every step forward your costs accelerate.

"The competition has been held for a number of years now but it is a new experience every time as something new is added each year," says Tove Holm Petersen.

"In the beginning the task was "just" to discover oil. Now you need to take in environmental concerns like spawn zones for fish. You are also required to decide whether you will try to insure yourself against losses from environmental risks. And the possibility to engage in partnerships with one or more competitors is another new element."

The 2010 version of the Danish PetroChallenge competition was sponsored by Maersk Oil and DONG Energy. Besides cash prizes for the best teams, the winning team is qualified for the international final in London.

All participating classes are invited to visit CERE.

Since its introduction in 2005, the Danish version of the international PetroChallenge competition has set a new record for participation each year. The image is from Sankt Annae Gymnasium, Copenhagen.
Photo: Sankt Annae Gymnasium

In Situ Burning in the Arctic

In situations with ice cover and at remote locations it may just not be possible to apply conventional methods for skimming and collection to Arctic oil spills. Here in situ burning is likely to be "the least of evils". A key factor is establishing the window of opportunity for the method depending on the type of oil and weathering conditions.

Despite general consensus on the need to develop a renewable energy future, according to International Energy Agency forecasts, oil and gas demand will increase over the next decades. As this is likely to stimulate growing interest in oil exploitation in the high North, readiness for taking care of major oil spills should become more in focus. The methods developed would of course also be relevant for handling minor oil spills i.e. from ships rinsing their tanks – a situation which, while not legal under international maritime conventions, is likely to become more frequent in the future since marine transportation will grow as Arctic sea ice cover is gradually decreasing due to global warming.

A key factor is establishing the window of opportunity for igniting an oil spill depending on the type of oil and weathering conditions. Photos: SINTEF

Key Findings for In Situ Burning

* The window of opportunity for the use of in situ burning in the Arctic can be larger than in the open sea.
* In situ burning has been tested and proven to be effective for the elimination of both free floating oil in ice and oil collected in fire resistant booms.
* Findings show that the presence of cold water and ice can enhance the effectiveness of in situ burning by limiting the spread of oil and slowing weathering processes.
* The field experiments verified in situ burning as an efficient technique, with a burn efficiency rate above 90 per cent.

Source: "Joint industry program on oil spill contingency for Arctic and ice-covered waters", SINTEF, 2010.

A joint industry program (JIP) led by Norwegian engineering consultants SINTEF address oil spill contingency for Arctic and ice-covered waters. A Ph.D. study by Janne Fritt-Rasmussen, DTU, has contributed to the program's in situ burning section.

In situ burning is one of the response techniques with the highest potential for removal of oil spills under Arctic conditions, especially in snow and dense ice. The effectiveness of in situ burning is verified by previous field experiments performed in the US, Canada and Norway, showing removal efficiencies over 90 per cent under the right circumstances.

High variation in windows of opportunity

"The main attraction of the method is that you don't need large scale equipment that will be logistically difficult to apply in a remote location. In the most favourable situations a proper igniter could actually be all you need," says Ph.D. Janne Fritt-Rasmussen. Her Ph.D. study was sponsored by the Committee for Scientific Investigations in Greenland (KVUG). Professor Arne Willumsen of the Arctic Technology Centre (ARTEK) at DTU was principal supervisor, while Professor Erling H. Stenby of CERE was co-supervisor.

The main concern in relation to Arctic oil spills would be a large spill of crude oil. However, crude oils are far from homogeneous. The project has investigated five crude oils from various fields and revealed a high degree of variability.

"If you look at a crude oil like Grane, having a high content of asphaltenes, you need to start ignition within just nine hours after the spill – and this is even under the most favourable weathering conditions – 90 per cent ice cover. For some other crude oils the window of opportunity stretches beyond 72 hours, which was the maximum length of our weathering experiments," tells Janne Fritt-Rasmussen.

Suddenly the moment is lost

The experiments clearly showed that the line between in situ burning being possible and impossible is very distinct. Establishing the window of opportunity for the method depending

> The main attraction of the method is that you don't need large scale equipment that will be logistically difficult to apply in a remote location. In the most favourable situations a proper igniter could actually be all you need.
>
> **Ph.D. Janne Fritt-Rasmussen.**

Oil spill contingency in Greenland

Increasing sea transport and possible oil and gas exploration are two challenges facing Greenland in the near future – both highlight the status of oil spill contingency. Presently 12 cities have oil spill equipment, each with a capacity to deal with a 20,000 liter spill. In comparison the spill from the tanker Exxon Valdez in Alaska, 1989, totalled close to 41 million liters.

In situ burning can not be compared to controlled incineration at a designated plant – the incineration will never be ideal and production of undesired by-products like soot can not be avoided. Still, in situ burning may be the least harmful alternative.

on the type of oil and weathering conditions is paramount to planning a given contingency operation. In the joint industry program SINTEF's Oil Weathering Model (OWM) has been supplemented with an in situ burning algorithm.

Besides using different crude oils the experiments have been carried out under different ice conditions – open water, 50 and 90 per cent ice coverage.

"As a rule of thumb Arctic conditions are relatively favourable to the method. Firstly, the presence of ice will dampen the energy of the system, leading to a slower mixing of oil and water (oil-in-water emulsion) which in turn will prolong the period where oil is able to burn. Secondly, the evaporation of the oil is slower than under warmer conditions, thus the amount of ignitable compounds left in the oil can be larger," Janne Fritt-Rasmussen explains.

Still, far from always will a cigarette lighter be enough to start the process.

"In our trials we used a "gelled" crude oil or gasoline added emulsion breaker as igniter. This would ensure that we in more cases would be able to ignite the oil locally. Whether the fire would keep on burning is of course another question – the answer would depend on the type of oil, the time since the spill, the weathering, the thickness of the oil spill and ice coverage."

Black smoke, bad PR

The experiments were carried out at three levels. Firstly, laboratory testing involving incineration of samples of 0.1 liter each. Secondly, 200 liter samples burned in situ under controlled conditions in the Svea fjord, Svalbard. Thirdly, close to full scale experiments burning two cubic metres of crude oil in the Barents Sea.

"Our experiments confirmed the high removal potential of the method," comments Janne Fritt-Rasmussen.

Still, she stresses that in situ burning will not avoid all potentially harmful environmental effects:

"Obviously, in situ burning can not be compared to controlled incineration at a designated plant – the incineration will never be ideal and production of undesired by-products like soot can not be avoided."

It is mainly soot that gives the smoke from in situ burning its distinct black colour.

"From a public relations point of view this is of course really bad. Nobody enjoys the sight of black smoke spreading across a beautiful white Arctic panorama. Still, as an engineer I believe that the method should be judged not by its appearance but by its efficiency compared to alternative methods," Janne Fritt-Rasmussen concludes.

"After all, we are talking about a situation where an accident has already happened. The key question will be how to minimize the harmful consequences."

Lars Jensen
PhD. Today works at CERE as Post Doc
Supervisor:
Nicolas von Solms

PhD Defense

Experimental Investigation and Molecular Simulation of Gas Hydrates

A combination of low temperature, high pressure and presence of water is known to provide conditions for formation of gas hydrates which may precipitate in pipes and production gear during oil recovery. This again may lead to production stops implying major economical losses. Presently large quantities of inhibitors, primarily methanol and ethylene glycol, are utilized to inhibit gas hydrate formation.

The thesis focuses on alternative methods for dealing with the problem.

It is possible to control formation of gas hydrates using small amounts of polymeric compounds (kinetic inhibitors) which instead of inhibiting the formation thermodynamically work by slowing the formation rate (kinetics). However, using kinetic hydrate inhibition requires a detailed knowledge of the nucleation and

PhD Defense

Migration of Plasticisers from PVC and other Polymers

In 2005 Danisco - one of the world's leading producers of ingredients for food - launched an alternative plasticiser for use in PVC for food packaging. The product, GRINDSTED SOFT-N-SAFE (SNS), is a fully acetylated glycerol monoester produced from castor oil. Extensive testing including animal testing has demonstrated absolutely no harmful effects from the product which is approved by the EU for food related use without any restrictions.

The main purpose of the thesis is to investigate migration of SNS and other plasticisers from PVC and polyolefin food package materials into foodstuff – especially into the four food simulants set by EU legislation.

It is shown how diffusion coefficients can be obtained by linear regression of experimental migration data plotted as the square root of time. This was done from plasticiser migration data of SNS, ACETEM 95 CO (Acetem) and Epoxidised Soybean Oil (ESBO) migrating from PVC and into iso-octane at 20°C, 40°C and 60°C. Using these experimentally obtained diffusion coefficients the migration was modelled using two analytical models with relatively good accuracy.

Furthermore using the finite element mesh method, migration was modelled with a diffusion coefficient dependent of the local plasticiser concentration. This numerical solution by the finite mesh method has also been used to model the migration of an antistatic additive to the surface of Low Density Polyethylene (LDPE) and Poly Propylene (PP). It was possible with a newly developed model to estimate the migration with very high accuracy. This result leads to the somewhat surprising conclusion that the controlling step in the migration of the additive to the surface was not the migration within the polymer bulk. This migration is probably due to a temperature dependent partitioning of the additive between the polymer bulk and the surface.

The possibility of using molecular dynamics calculations to estimate the partition coefficients of additives between polymers and foodstuff was also investigated. The development of the methodology was done against experimental data of a system composed of a hydrophilic or hydrophobic additive between LDPE and different water/ethanol mixtures. The calculated partition coefficients of different additives between LDPE and water/ethanol were correlated with high accuracy against experimental data.

To extend the methodology to acetic acid systems (EU food simulant B), it was chosen firstly to investigate the predictive capabilities of the chosen force fields for pure acetic acid and acetic acid / water mixtures. None of the force fields were able to predict satisfactorily the density of acetic acid / water mixtures, and the over-prediction of the heat of vaporization turned out to be caused by the data used for fitting the force fields parameters.

Overall it can be concluded that a full prediction of migration in polyolefins can be obtained using the numerical solution by finite element mesh together with diffusion coefficients obtained from the Piringer model and partition coefficient by molecular dynamics.

Rasmus Lundsgaard
PhD
Today Post Doc with CERE and NKT Flexibles
Supervisor: Georgios Kontogeorgis

growth of gas hydrates and how these processes are influenced by pressure and temperature in relation to the phase equilibria and not least kinetic inhibitors.

The thesis investigates phase equilibria, nucleation and growth of gas hydrates using experimental approaches and theoretical models. Monte Carlo simulation – a molecular simulation tool for studying complex fluid systems – is shown to be very useful for calculating the temperature and pressure dependence of the hydrate melting point, the hydrate equilibrium composition and the hydrate melting enthalpy. These results are encouraging since they suggest that molecular simulation may be suitable for predicting hydrate properties which are very difficult to access experimentally.

The thesis includes a class of biological molecules often referred to as antifreeze proteins. It is shown that antifreeze proteins – so named because they inhibit ice formation in certain plants and animals – are very effective kinetic hydrate inhibitors and in some cases even better than some of the synthetic inhibitors used in the oil industry today. Since antifreeze proteins are regarded as environmentally benign, as opposed to synthetic inhibitors, they may contribute to making the production of oil and gas greener.

Glycols, Salts and Mercaptans in Gas Processing

Ever more complex mixtures are covered by theoretical and experimental work under CERE's Chemicals for Gas Processing (CHIGP) project.

Traditionally cubic equations of state have been applied to describe phase equalibria in an oil-gas mixture. Cubic equations of state are relatively simple and hold an outstanding track record within gas-liquid phase equilibria solutions related to oil recovery. Current oil recovery does however depend on a range of chemicals needed to facilitate production, i.e. polymers, surface active substances, emulsion breakers and hydrate inhibitors.

Adjusting traditional equations of state to cope with the complex mixtures found under recovery today is the main justification of CERE's joint industrial project Chemicals for Gas Processing (CHIGP). Current participants are Statoil, GASSCO, BP, Maersk Oil and DONG Energy, who joined in 2010.

The major purpose of the project is to develop and maintain a rigorous thermodynamic model, the CPA (Cubic-Plus-Association) equation of state. CPA is a model useful for thermodynamic calculations for mixtures of relevance to the petroleum and chemical industries e.g. mixtures of oil and gas with gas hydrate inhibitors (methanol, glycols) and organic acids.

"Such polar and hydrogen bonding compounds are difficult to handle with conventional models used in oil industry like cubic equations of state and CPA offers a successful alternative and is a good compromise between accuracy and simplicity," comments Professor Georgios M. Kontogeorgis, CERE, head of CHIGP.

> Hydrogen bonding compounds are difficult to handle with conventional models used in oil industry like cubic equations of state. CPA offers a good compromise between accuracy and simplicity.
>
> **Professor Georgios M. Kontogeorgis, CERE, head of CHIGP**

Salts in oil-related mixtures

2010 was the project's 8th consecutive year.

"In addition to extending the model to new mixtures of industrial and scientific significance, robust algorithms for complex thermodynamic calculations and parameter estimation are being developed and new experimental measurements are being carried out when necessary in order to support the model development. Such measurements are often being carried out in collaboration with industrial partners of the CHIGP consortium," says Georgios M. Kontogeorgis.

Understanding gas-liquid and liquid-liquid equilibria involves considerable economical and environmental interest. Examples are methanol and ethylene glycol which are both used in large quantities to inhibit hydrate formation. The key issue is finding the proper level of inhibitors;

using just enough to do the job.

A new Ph.D. project (Bjørn Maribo-Mogensen) will further extend CPA to mixtures with electrolytes especially with the purpose of describing the effect of salts in oil-related mixtures, including those containing gas hydrate inhibitors and salts.

Also, new thermodynamic measurements for oil mixtures in presence of water and glycols and dew points for synthetic and real natural gas mixtures have been conducted during 2010. All these measurements have been carried out at Statoil's research center in Trondheim, Norway.

Successful inclusion of acid gases

A new post-doctoral grant for Dr. Javeed Awan obtained from the Danish Research Council is on a topic connected to the CHIGP project; measurements and modeling for mixtures containing mercaptans, which are sulfur compounds of importance to oil industry. These measurements are quite difficult and require special equipment and safety regulations. They are currently being carried out by Javeed at Ecole de Mines in France with which CERE is collaborating in this project.

"In addition to the above mentioned projects, a very significant activity during 2010 has been the modeling of mixtures containing acid gases (CO_2, H_2S), hydrocarbons, water and other polar chemicals. Dr. Ioannis Tsivintzelis has carried out this work that illustrated that CPA can be successfully used for such systems over extensive temperature and pressure ranges," Georgios M. Kontogeorgis explains.

More demanding has been the modeling of mixtures with aromatic acids such as those involved in terephthalic acid production. This work is in progress.

Reaching Out

Results from the project are disseminated via CERE's web-site www.cere.dtu.dk and a special project sub-site. The deliverables include software in form of CAPE-OPEN compliant modules and user-models for the ASPEN process simulator. In this way the results can be used by industry almost as soon as they are produced. Moreover, the results are presented in progress meetings held twice per year; 14 meetings have been held since 2003. The last one took place in December 2010.

Foto: Øyvind Sætre/Gassco

Norway Prepares to Pioneer CO_2 storage

As one of the world's first countries, Norway is considering to build a full-scale carbon capture plant with subsequent offshore storage. Preparations involve equations of state developed in the CHIGP project.

> We plan to use equations of state developed in the CHIGP project to operate a system of offshore pipelines for carbon dioxide storage, which is currently under development.
>
> **Tormod Spangelo, Senior Project Engineer, Gassco**

The Ministry of Petroleum and Energy (MPE) of Norway has commissioned Gassco to prepare transport solutions for planned carbon capture from gas-fired power stations at Kårstø and Mongstad.

"We plan to use equations of state developed in the CHIGP project to operate a system of offshore pipelines for carbon dioxide storage, which is currently under development," Tormod Spangelo, Senior Project Engineer, Gassco, informs.

Owned wholly by the Norwegian state, Gassco is the operator for the integrated system for transporting gas from the Norwegian continental shelf to other European countries.

Beginning in 2007, Gassco has carried out conceptual studies for carbon transport from the Naturkraft power station at Kårstø and the Mongstad refinery to long-term storage on the Norwegian continental shelf. Solutions studied cover pipelines from Kårstø and Mongstad to the Utsira South formation in the Sleipner area and in the Johansen formation further east.

Gassco joined the CERE Industry Consortium in 2008 with special interest for the CHIGP project.

"We may find our participation useful in other cases as well, and it always is an inspiration to work with the academic community, but here and now it is mainly the carbon dioxide related projects that we focus on in relation to CHIGP," says Tormod Spangelo.

The time frame for the Norwegian carbon storage program has been extended a few times. A realistic year for full-scale implementation is likely to be 2018.

Gassco

Gassco was established by the Norwegian state May 2001 and soon after took over the operatorship for all gas transport from the Norwegian shelf.

During 2009 Gassco delivered a total volume of 96.6 billion cubic meters of gas to receiving terminals plus a total volume of 8.65 million tonnes of other products - primarily ethane, propane, butanes, naphtha and condensate (light oil). Gassco does not make a profit or a loss from its own operations. The cost of operating the transport system is met by its users through tariff payments.

PhD Defense

Extension of Association Models to Complex Chemicals

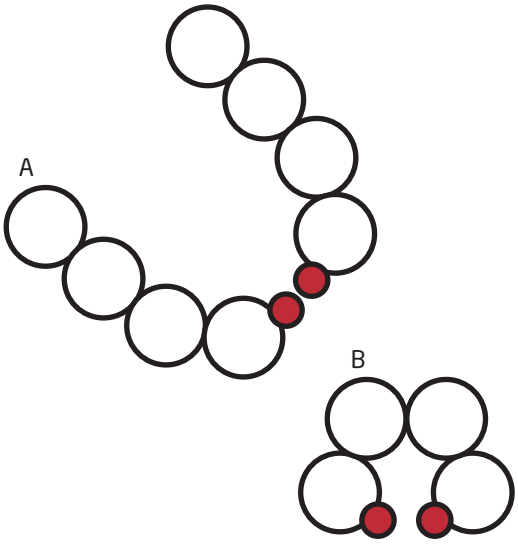
Ane Søgaard Avlund
PhD
Supervisor: Georgios Kontogeorgis

Thermodynamic models are important tools in any chemical process design in order to satisfy product specifications, ensure and optimize production and processing. Whether it is in the design of a distillation column, a flash or a pipeline it is important to be able to determine the thermodynamic properties of the fluids and solids involved. Experimental data is usually available for these properties at limited conditions, and are often expensive and time consuming to conduct. A thermodynamic model, which allows you to extrapolate or even predict the experimental data at other pressures and temperatures than those where data is available, is therefore very desirable. If a reliable model is available it is possible to determine the bubble point pressure, the critical solution temperature, the composition of coexisting phases, the energy required in a certain step in the process and many other factors.

The thesis is focused on modelling compounds of interest to the petroleum industry using equations of state. The petroleum industry uses a number of chemicals at various stages in the oil production; i.e. glycol ethers are used in chemical flooding of oil reservoirs to enhance oil recovery by decreasing interfacial tension between oil and the displacing fluid, normally brine. Glycols or methanol are used to avoid gas hydrate formation in off-shore process equipment and transmission lines. Alkanolamines are used for removal of acid gases like CO_2 and H_2S from natural gas streams.

A common feature for the compounds mentioned is their ability to form hydrogen bonds – they are so called associating compounds. Some of the compounds like glycols and surfactants are especially complex as they can form hydrogen bonds inside the same molecule as well, a phenomenon called intramolecular association. The subject of the thesis is application of SAFT (Statistical Association Fluid Theory) type equations of state to complex mixtures relevant to the petroleum industry, and to extend these theories to compounds which exhibit intramolecular association. Mainly two equations of state are used; CPA (cubic plus association) and sPC-SAFT. Both models have been used for alkanolamines, whereas a novel theory for including intramolecular association in SAFT has been developed.

The results are promising for the glycolethers considered. It has however been shown that for engineering models like CPA and SAFT, parameter estimation is at least as important as improvement in theory. While different parameter sets are found to give similar pure component vapour pressure and liquid density results, very different mixture results are obtained. The performance of the theory therefore depends significantly on parameter estimation. Nevertheless, CPA and sPC-SAFT are powerful models for phase equilibrium calculations in complex mixtures containing hydrogen bonding compounds, not just water and alcohols, but also multifunctional ones like glycolethers and alkanolamines.



A common feature for the compounds investigated is their ability to form hydrogen bonds – they are so called associating compounds (A). Some of the compounds like glycols and surfactants are especially complex as they can form hydrogen bonds inside the same molecule as well, a phenomenon called intramolecular association (B).

Innovative Techniques for Carbon Capture

From a strictly technical point of view it has been possible for some time to produce power and heat from coal without notable carbon dioxide emissions; technology able to extract carbon dioxide from flue gas from coal fired power plants already exist. However, a dual challenge persists. Firstly, costs need to decrease to a level where large scale introduction is feasible. Secondly, doing the right thing for climate shouldn't introduce new types of environmental problems. While development and optimization of proven technologies continue, a range of innovative approaches has entered the playing field.

Governments world wide demonstrate increasing interest in carbon capture and storage (CCS). This is mainly due to the fact that despite general consensus on the need to develop a renewable energy future, according to International Energy Agency (IEA) forecasts, coal consumption will continue and probably even increase over the next decades. This has led to interest in a range of alternative methods for carbon capture.

"The modest result from the UN conference on climate change in Copenhagen, December 2009, hasn't exactly favoured carbon capture in general, as we didn't get a global price on carbon emissions. But then again, this has taken some of the urgency out of the field. This in turn may give some of the techniques that are really innovative - but also quite far from realization -time to enter the playing field if they can prove themselves efficient," comments Assistant Professor, Ph. D., Philip Fosbøl, CERE.

One group of possible alternatives relate to radical changes in the very combustion process at a coal fired plant. These ideas, the so called oxy fuel process being the most notable, are beyond the scope of capture research at CERE. Instead the centre's research focuses on chemical absorption methods based on capturing carbon dioxide by means of a solution where an appropriate substance – a solvent – is dissolved in water. In a later step the captured carbon dioxide will be released from the solution while the solvent is recycled back into the capturing zone. The carbon dioxide captured will be stored in a suitable geological structure.

> Some of the capture techniques that are really innovative may still have time to enter the playing field. As to which technique will end up as the best. The ball is up in the air and it is harder than ever to predict where it will land.
>
> **Assistant Professor, Ph. D., Philip Fosbøl, CERE.**

Alkanolamines - the classic option

Capturing carbon dioxide by chemical absorption from a mixture containing other gases is by no means a novel exercise. Carbon dioxide is a useful product in a range of industrial processes and

methods for producing it have existed for many years. Also, in submarines capture equipment is crucial as otherwise the expiration of carbon dioxide by the crew would gradually make it impossible to maintain life in the vehicle's atmosphere.

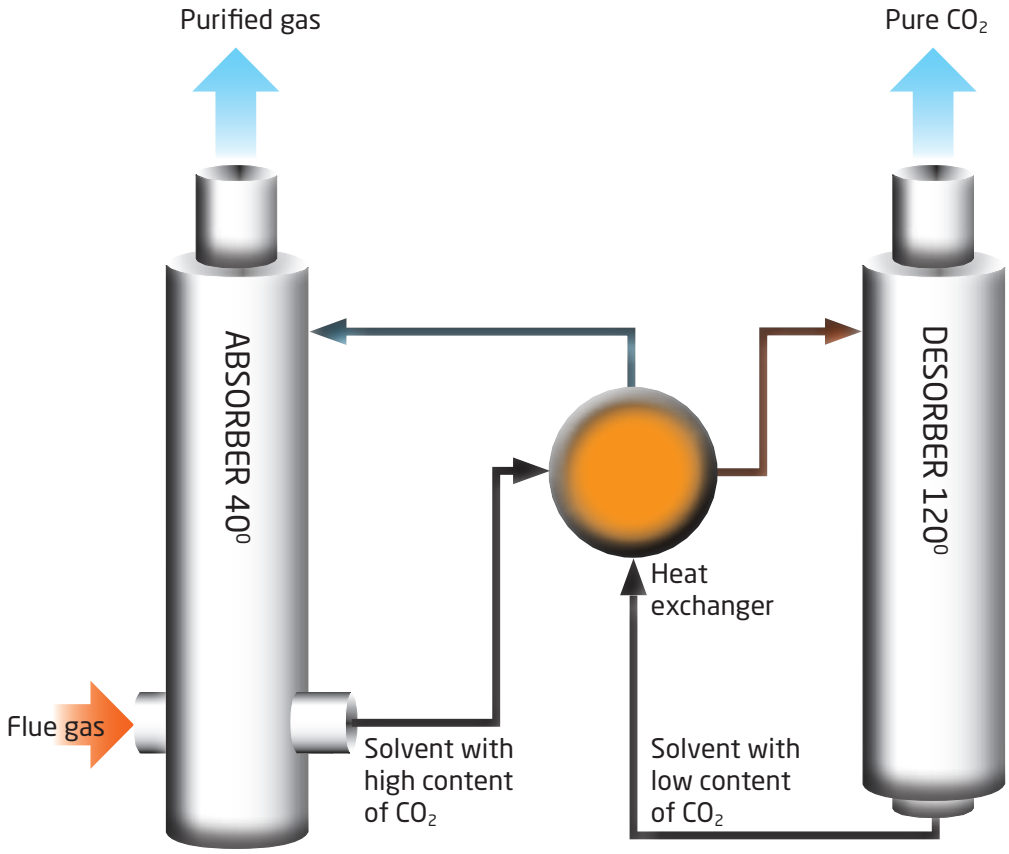
What characterizes a suitable solvent? Firstly, it should of course be able to capture carbon dioxide efficiently – meaning both an ability to capture a large quantum in relation to its own volume and an ability to do so quickly. On the other hand the solvent shouldn't bond too tightly to carbon dioxide which will need to be freed later in the process allowing for the solvent to engage in renewed capture. Finally, to minimize the amount of solvent lost before, during and after the capture process the solvent needs to be stable under process conditions.

As properties in demand are plentiful – and some of these even contradictory – no solvent can be absolutely ideal. The challenge is to find the best compromise. Most techniques presently used for carbon dioxide capture are based on amines – derivative compounds of ammonia in which the hydrogen atoms are replaced by one or more organic hydrocarbon radicals. The standard choice would be alkanolamines – by far the technique with the longest track record within carbon dioxide capture and still one of the techniques contesting for becoming the large scale capture method of the future.

Why look for alternative solvents?

However, two drawbacks related to alkanolamines have come to attention.

The first concern is cost. The present version of the technique is estimated to result in a 25



Carbon dioxide may be captured by means of a solution where an appropriate substance – a solvent – is dissolved in water. In a later step the captured carbon dioxide is released from the solution while the solvent is recycled back into the capturing zone.

per cent increase in the consumer's price for electricity. Ultimately, it is a political decision whether a rise in prices of this magnitude is acceptable in view of combating climate change, but here and now such an increase would seem to constitute a barrier. One should also remember that the figure only covers capture expenses – not storage and other related costs. A further concern is the fact that since alkanolamine capture has a long track record it is not very likely to find further process optimizations that could reduce costs significantly.

The second concern is environment. Unfortunately the conditions present during carbon dioxide capture from a power station's flue gas lead to some degree of alkanolamine decomposition. For one thing this is undesired simply because one loses solvent, which in turn adds to costs. Worse, however, is the fact that some of the decomposition products are quite chemically reactive and toxic. In other words people living in proximity to the power station may end up with an environment and health problem if these problems are not resolved.

While the quest for solutions both to the cost challenge and the environmental problem is ongoing and may turn out successful it seems only natural to consider alternatives to alkanolamines.

Chilled ammonia, ionic fluids

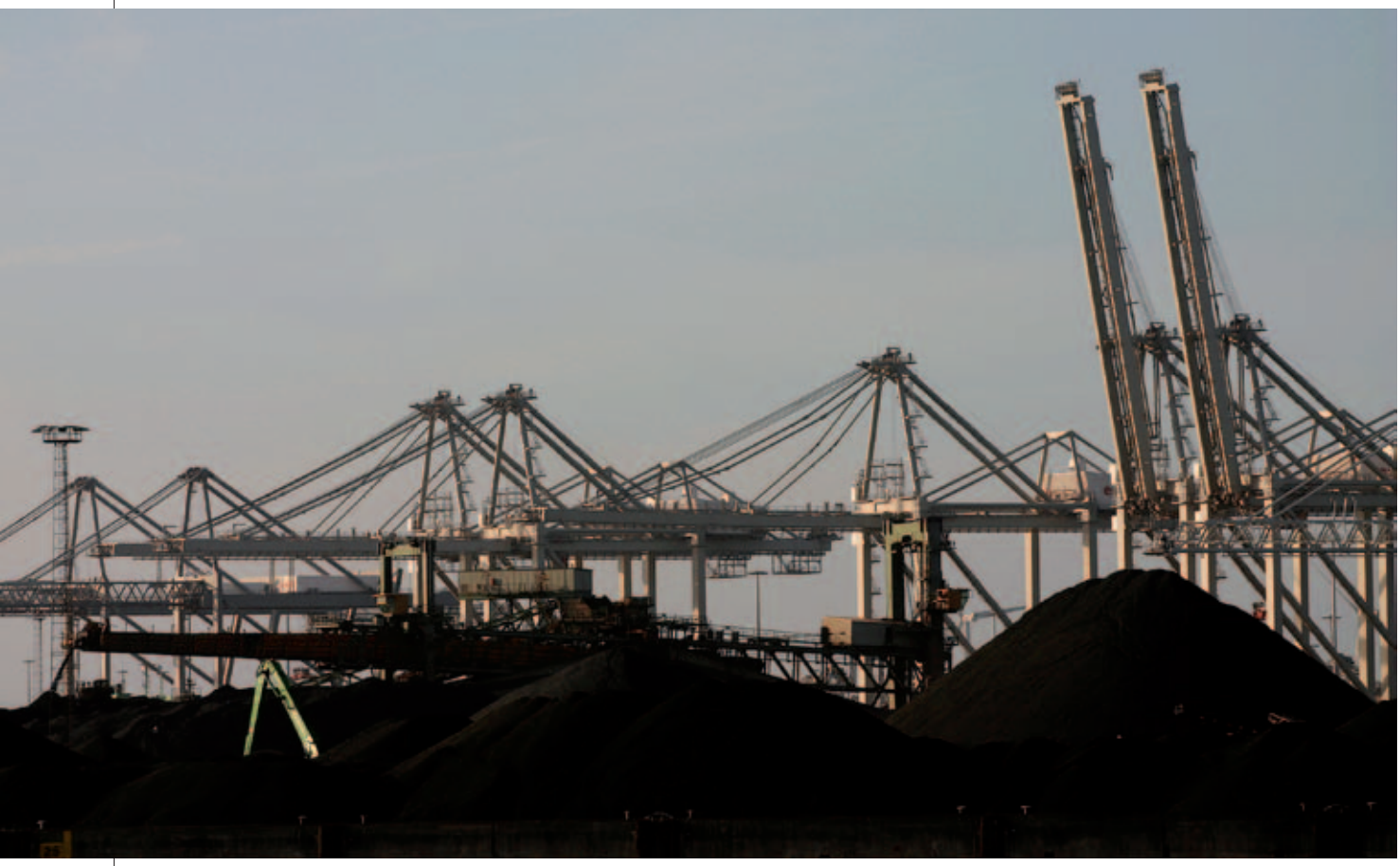
One alternative is the "chilled ammonia" process. Chemically speaking ammonia is a suitable solvent for carbon capture, but at room temperature ammonia would vaporize from the solution. Therefore ammonia has to be added in chilled form. The cooling represents some practical challenges plus extra costs as it requires energy. Still, the chilled ammonia process is considered well advanced and one of the runner ups to challenge alkanolamine processes in the near future.

Another CERE project – carried out in cooperation with DTU Chemistry - address ionic fluids. Professor Rasmus Fehrmann and colleagues at DTU Chemistry have previously been successful in utilizing ionic fluids for sulphur dioxide capture. The group is currently looking into the ability of the same substances in capturing carbon dioxide, while cooperating with CERE in attempts to design and synthesize novel ionic fluids that are fit for carbon capture.

"An ideal concept based on ionic fluids would have both sulphur dioxide and carbon dioxide capture within the same process. This would optimize efficiency and economic feasibility," comments Philip Fosbøl of CERE.

Initial studies are promising, he adds:

Despite general consensus on the need to develop a renewable energy future, according to International Energy Agency (IEA) forecasts, coal consumption will continue and probably even increase over the next decades. This has led to interest in a range of alternative methods for carbon capture. Photos: Bigstock



"But until you have actually built a full scale plant and demonstrated high efficiency and low use of energy for the process, you still have to look at ionic fluids as basic research."

Capture inspired by biology

A novel area which has attracted large interest over short time is amino acid based capture methods. The first articles suggesting use of amino acids for carbon capture are less than a decade old.

"In just a few years a large number of research projects have been initiated. But unfortunately due to the huge commercial potential most of the results remain unpublished. So if you want to work in this field you will have to do a broad range of experimental work as the opportunities to just look up things are scarce," says Ph.D. Student Benedicte Mai Lerche, CERE.

Amino acid based carbon capture can be described as a bio-mimetic process as it resembles the way carbon dioxide is captured by haemoglobin and other proteins in our blood. Amino acids may be produced synthetically or by fermentation or by hydrolyses of natural proteins.

"It seems likely that one of more techniques based on amino acids can be proven better compared with traditional alkanolamine carbon capture. Firstly, amino acids are naturally occurring substances. Secondly, they are stable under exposure to oxygen. Thirdly, we have a large variety of amino acids capable of capturing carbon dioxide. As we have a wide range of selection, likeliness of finding one or more really suitable amino acids is good," says Benedicte Mai Lerche.

She stresses that a great deal of further research is required:

"We need to assure that the use of amino acids for this purpose does not introduce unforeseen harmful effects. Also, we need to test physical and chemical properties of relevant amino acids under realistic process conditions."

In pilot plants around the world using alkanolamine solutions or similar methods process temperatures are typically around 120 degrees C.

"One would think this to be too hot for organic compounds like amino acids but actually some amino acids remain stable. Others can't tolerate this kind of heat, but even so - if the temperature could be lowered somewhat they could become candidates," Benedicte Mai Lerche comments and sums up:

"In my view amino acids are likely to be attractive carbon capture candidates as they may honour the technical demands while not introducing new types of environmental or health concerns."

Innovative capture goes European

A number of even more recent ideas are investigated through European Union research program "iCap"; where the "i" is for "Innovation". While Norwegian university NTNU is the overall coordinator, CERE coordinates one of five work packages. The work package involves thermodynamic modelling.

"In other words we are the link between experimental results and later simulations done by other partners in the program," Peter Jørgensen Herslund, Ph.D. Student at CERE, explains.

He is also involved in the details around one of the innovative techniques investigated under the European program; namely using gas hydrates for carbon capture. Gas hydrates are substances resembling snow or ice consisting of water and light hydrocarbons. In many contexts – i.e. oil and gas exploration – gas hydrates are highly undesired, but recently the idea has come up to use them for carbon capture.

Formation of gas hydrates is in some ways similar to formation of ice. While a layman thinks of ice formation as always taking place at 0 degrees C, the professional knows that changes in pressure will move the freezing point. Also, the point can be influenced by adding chemical substances to the water. Often inhibitors, primarily methanol and ethylene glycol, will be used to move the freezing point downwards. The point of gas hydrate formation can be lowered in the

same way – and it can also be raised.

"While some of my colleagues here at CERE are looking for ways to prevent gas hydrate formation, I am interested in achieving the exact opposite. I can use a lot of their experiences but of course the chemicals that interest me have properties that are very different to those that would interest them," says Peter Jørgensen Herslund.

Under standard conditions high pressure will be needed to compress flue gas at a power station to a degree where gas hydrate formation may occur.

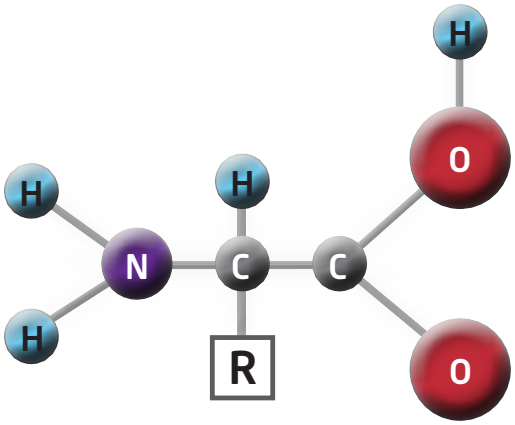
"High pressure equals high costs so we are looking into ways to have hydrate formation at not quite so high pressure," Peter Jørgensen Herslund states, while adding that the high pressure is not entirely undesired:

"The carbon dioxide captured would need to be compressed later anyway when it is to be stored. By doing the initial capture under pressure we save this later step."

True price of solvents is a joker

Instead of gas hydrate inhibitors, one would add substances that promote hydrate formation. In his research, Peter Jørgensen Herslund uses THF – Tetra-Hydro-Furan – a substance with proven ability to raise the point of gas hydrate formation:

"Unfortunately the environmental and work hazard properties of THF are not suitable for introducing it into large scale carbon capture. We use THF to model the process. We want to see whether it is possible to capture carbon dioxide at the required efficiency and to release it again in a way that allows for the THF to be freed and recycled for renewed capture. If we manage this, as we hope to demonstrate, we will look for an alternative substance that can also raise the point of gas hydrate formation but doesn't cause environment and health concerns."



A relatively novel technique for carbon capture is using amino acids as solvents. The illustration shows the structure of an amino acid. The "R" symbolizes a side-chain which is specific for each amino acid.

The European program also covers a number of other innovative approaches to carbon capture. As the program is quite new – it was initiated in February 2010 and runs for four years – and involves a large number of European research institutions, it is still early to say which concepts will come out and how successful they will be. It is also difficult to estimate how these innovative ideas will do against more mature solutions that are closer to practical implementation. A further joker is uncertainty over the true price of some of the solvents investigated in innovative projects. Currently a number of these substances – i.e. certain amino acids - are extremely expensive but it seems likely that they can be produced at much lower costs if they come in demand in relation to large scale implementation of capture technology.

CERE's Philip Fosbøl sums up:

"As to which technique will end up as the best the ball is up in the air and it is harder than ever to predict where it will land."

PhD Defense

Post-Combustion Capture of CO_2 from Fossil Fueled Power Plants

Leila Faramarzi
PhD
Today works at
Doosan Babcock, UK
Supervisor:
Georgios
Kontogeorgis

Carbon capture and storage (CCS) is a promising option for limiting atmospheric CO_2 accumulation as it can be implemented without changes in energy supply infrastructure and without major changes to the basic process of power generation.

A well established process for separation of acid gases from gaseous streams is absorption by a liquid media. The liquid media are often aqueous alkanolamine solutions or other fluids with alkaline character, such as chilled or ambient temperature ammonia.

One useful feature of amine processes is that they are applicable at low concentrations of CO_2 encountered in power plant flue gases. Moreover, chemical absorption using amines is a well established process with years of experience around it, and it can be retrofitted to existing power plants. Thus, alkanolamine-based post-combustion capture (PCC) is considered state of the art technology for CO_2 removal from flue gases. The most commonly used amine is MEA, monoethanolamine. The underlying principle for MEA-based PCC is the exothermic, reversible reaction between a weak acid and a weak base resulting in formation of a soluble salt.

The main objective of the thesis was to develop an alkanolamine-based CO_2 capture process design model and validate it against experimental data from literature. An in-house model, extended UNIQUAC, was applied to estimate various thermodynamic properties of the alkanolamine systems required. In addition, the model proved capable of representing different types of thermodynamic properties of the aqueous CO_2-alkanolamine systems in a broad range of conditions using only one unique set of parameters. It is shown that extended UNIQUAC can accurately represent physical and chemical equilibria over a wide range of conditions.

Further, a rate-based steady state model proposed by Gabrielsen et al. (see IVC-SEP Annual Report 2007) for the design of CO_2- 2-amino-2-methyl-propanol (AMP) absorbers was adopted and improved for design of a CO_2- monoethanolamine (MEA) absorber. The model was successfully applied to CO_2 absorber packed columns and validated against pilot plant data with good agreement.

PhD Defense

Design, Development and Testing of New Experimental Equipment for the Measurement of Multiphase Equilibrium

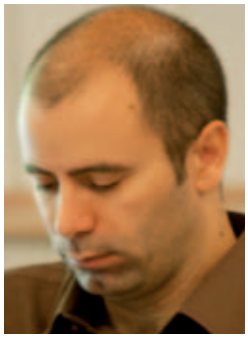
Measurements of phase equilibria are important to a number of applications within energy resource engineering and related fields. The thesis is focused on measurements of multiphase equilibria in hydrate inhibitor systems relevant to oil and gas production and on measurements of multiphase equilibria relevant to carbon dioxide capture.

Two experimental set-ups were built for these two purposes at the laboratories at CERE-DTU. The nature of the work was characterised by a broader perspective – it is possible to guidance for future experimental work with these equilibrium cells. The commissioning of the two apparatus opens a range of opportunities for different projects.

An aspect worth mentioning – especially in times where resources are limited – is the low cost of the equipment. The first analytical apparatus was planned, designed and built with an overall cost several times less than commercial solutions available. Furthermore, this allows a higher degree of customisation, entailing a fewer compromises - always inevitable where commercial equipment is concerned. The second apparatus constitutes an example of reuse of decommissioned equipment, with substantial improvements in set-up quality at very low cost.

The thesis contains a detailed description of design and selection of parts. Furthermore, all tests are presented, including the less successful ones that often occur in experimental work, but seldom get published. This allows the thesis to be used as a guide for future experimental work.

Besides the developed set-ups, the thesis contains a review of experimental methods available for phase equilibria measurements. In a complementary part of the work, modelling was performed, mainly by verification of the applicability of the simplified PC-SAFT equation of state, by the correlation of a number of binary systems and in a second stage in the prediction of the equilibrium phase compositions in a quarternary system studied experimentally.



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First landmarks under the CERE flag

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2010, the first full year as Center for Energy Resources Engineering, saw a number of research breakthroughs, notable contributions in funding and media attention.

As we became Center for Energy Resources Engineering (CERE) by late 2009, the change of name was more than just symbolic. Supported by a strategic decision by DTU's top management, we were able to strengthen existing strongholds within thermodynamics and associated disciplines of our Faculty, while including new research fields relevant to our core activities. As an example, the inclusion of geophysical and geological Faculty members was a natural extension of our research within oil and gas exploitation processes, Enhanced Oil Recovery and Carbon Capture and Storage.

As CERE we refer directly to DTU's management and enjoy an enhanced freedom to put our academic resources to use where we identify the highest degree of relevance. Also we enjoy enlarged possibilities for including academic resources elsewhere within DTU as part of ad-hoc research projects.

Already in CERE's first year we have seen a fine example of new interdisciplinary activity generated by the extended scope of the centre. A project on geothermal energy has attracted a funding of close to 2.0 million EUR from The Danish Council for Strategic Research. The project is headed by geologist, Associate Professor, Dr. Sc., Ida Lykke Fabricius, who became a Faculty member at CERE's start. The same was true for geophysicist, Professor Klaus Mosegaard, who will contribute to the project on geothermal energy while raising the centre's profile within petroleum engineering science and education.

The project on geothermal energy will involve a number of other CERE Faculty and industrial Consortium members. We expect the project to raise the understanding of this relatively novel and renewable energy source in general and its potential in Denmark specifically.

Innovative Capture Technologies

Another field where we see great potential for synergy between CERE's original and new Faculty members is Carbon Capture and Storage (CCS). While the center has a long tradition

for research within Capture, our new academic resources may contribute strongly to the Storage field.

A major event for our CCS involvement was the introduction of the European Union research program "iCap" (where the "i" is for "Innovation"). CERE coordinates one of the program's five work packages. The work package involves thermodynamic modelling.

The European program also covers a number of other innovative approaches to carbon capture. The program, initiated in February 2010 and running for four years, involves a large number of European research institutions. It will broaden the scope of our CCS activities and include novel concepts.

Enhanced Oil Recovery

An indisputable highlight for us in 2010 was the role as host for a Society of Petroleum Engineers symposium entitled "EOR: Averting another oil crisis". At the symposium, held August 18th, speakers from The Danish Energy Agency, Maersk Oil, DONG Energy, ConocoPhillips and Schlumberger covered plans for Enhanced Oil Recovery (EOR) in Denmark, experience in Norway and also global EOR offshore experience.

In addition, CERE's participants (Erling H. Stenby, Ida L. Fabricius and Wei Yan) presented findings from the project "Enhanced Oil Recovery through CO_2 Utilisation" performed in collaboration with engineering consultancy group GEO and Geological Survey of Denmark and Greenland (GEUS). The project was supported by the Danish National Advanced Technology Foundation and DONG Energy. Our findings suggest that carbon dioxide flooding seems to be an EOR method which is surprisingly efficient when applied to tight chalk reservoirs. This is particularly interesting for Denmark, as roughly half of known oil reserves in the Danish part of the North Sea are found in chalk with extremely low permeability from the so called Danien period, but also of broader international interest.

The EOR CO_2 findings and the SPE symposium in general attracted wide interest from industry, academia, government and administration as was also illustrated by considerable media coverage.

Proteins as hydrate inhibitors

Again, in 2010, we were able to maintain a high level of Ph. D. research. No fewer than se-

ven degrees based on high quality thesis were completed this year, just as eight fresh Ph.D. students, already looking promising, have set out.

A Ph.D. project receiving extensive media coverage in 2010 was Lars Jensen's results on proteins as gas hydrate inhibitors. His thesis, supervised by Associate Professor Nicolas von Solms, suggests that naturally occurring proteins found in organisms like bark beetle, meal worm and Arctic fish species can replace large quantities of gas hydrate inhibitors like methanol and glycol, which is needed presently to secure oil and gas recovery under cold and high-pressure conditions. Under fierce competition the research group was able to attract a 0.9 million EUR grant from The Danish Council for Independent Research / Technology and Production Sciences. This will ensure continued research in the field, which already involves cooperation with members of CERE's industrial Consortium.

These new breakthroughs have been achieved without jeopardizing existing strongholds of CERE. For instance, 2010 was the 8th consecutive year of the CHIGP project (Chemicals for Gas Processing). Adjusting traditional equations of state to cope with the complex mixtures found under recovery today is the main justification of this joint industrial project. Current participants are Statoil, GASSCO, BP, Maersk Oil and, last but not least, DONG Energy, who joined in 2010.

The CHIGP project maintains and develops the thermodynamic model CPA (Cubic-Plus-Association) for thermodynamic calculations of mixtures of relevance to the petroleum and chemical industries e.g. mixtures of oil and gas with gas hydrate inhibitors (methanol, glycols) and organic acids. The project is a Joint Industry Project, which maintains a high degree of cooperation with members of CERE's industrial Consortium, and a new enquiries for participation are of course always welcome.

Summer school tradition

The annual Discussion Meeting of CERE took place for the 31st time from 9-11 June at Loskolen in Elsinore. The attendance from our member companies was excellent and the interaction between colleagues and external participants as usual very fruitful. We will of course continue this significant yearly event for the Center.

Another proud CERE tradition of organizing advanced summer schools within thermodynamics was maintained in 2010 by Professor Michael L. Michelsen – heading the "Advanced Course on Thermodynamic Models: Fundamentals & Computational Aspects" from August 9th till August 27th – and by head of CHIGP, Professor Georgios Kontogeorgis, organizing "Advanced Course on Molecular Simulation of Complex Chemical Systems with Emphasis to Practical Applications" from June 28th till July 9th - Professor Vlasis G. Mavrantzas of University of Patras & FORTH-ICE/HT, Greece, was co-organizer of this course.

Both summer schools were - as always - extremely well attended, and the tradition will be continued in 2011.

For a group of ten CERE Faculty and Ph.D. students one of the year's most memorable moments was their participation in the world's

largest applied thermodynamics conference, the PPEPPD. The conference is held once every third year, the 2010 version took place in Jiangsou, China. As attendance is by invitation only, the fact that CERE was allowed to send a delegation of this size to present the newest results from the group was an honour in itself.

Singing in harmony

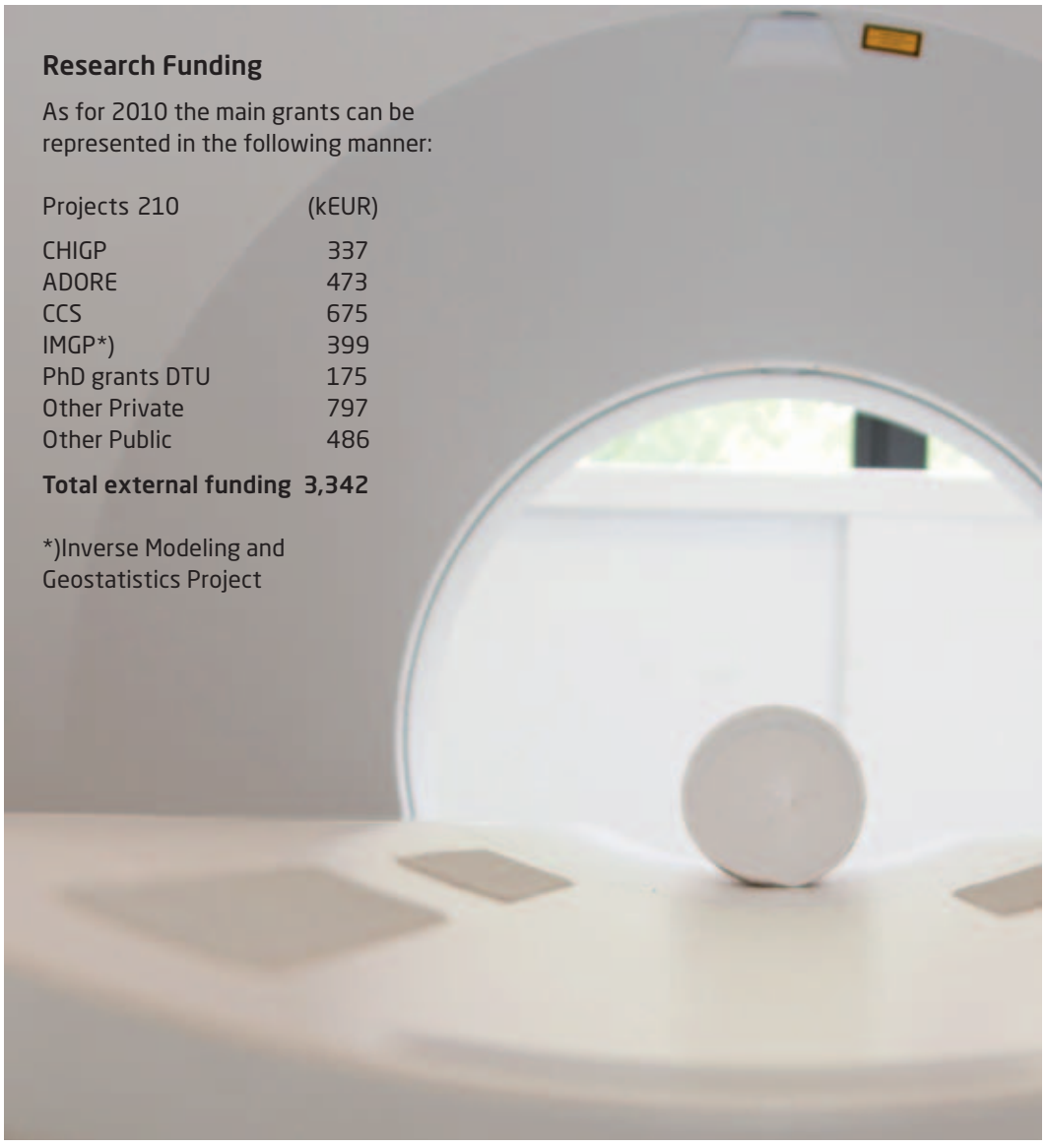
On a personal note I may add that the year was special as I accepted the dual challenge of heading both CERE and the Department of Chemistry at DTU – an interesting and in many aspects highly relevant broadening of my significant interest in research management.

Speaking of notes, in CERE we were able to enjoy singing voices during two weeks of November. For a new entity, as the center is, we found teambuilding to be important. While hopefully not insulting the sworn believers in wilderness survival courses, we opted for conductor Peter Hanke and his ensemble "Via Madrigali" to demonstrate the importance of the contributions of the individual singer to the overall performance of the ensemble over a number of sessions and exercises. A fruitful lesson we can take with us into our second full year as the CERE ensemble.

Research funding

As a university research group our job objective is to spend all of our money on research. Not at once but over time we can spend the funding we receive on research related activities. No bonuses to the management and no dividends to the investors. We try to be as good as possible at spending with the objective to maximize the production of research results and highly skilled researchers at PhD and Post Doc level.

The research carried out in CERE is funded by grants from a number of public and private sponsors. During 2010 our external research funding has increased to a total budget of EUR 3.3 million.



Research Funding

As for 2010 the main grants can be represented in the following manner:

Projects 210	(kEUR)
CHIGP	337
ADORE	473
CCS	675
IMGP*)	399
PhD grants DTU	175
Other Private	797
Other Public	486
Total external funding	**3,342**

*)Inverse Modeling and Geostatistics Project

Conference contributions & Invited speakers

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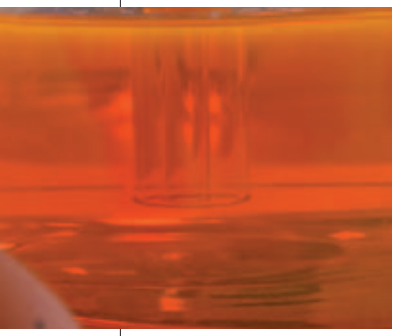

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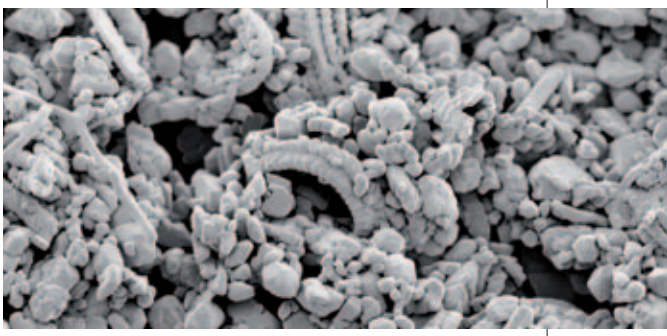

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Tsivintzelis, I., Kontogeorgis, G.M., Michelsen, M.L., Stenby, E.H. 2010: "Recent Applications of the CPA Equation of State" (Poster presentation), Special Symposium: 20 years of the SAFT equation: Recent advantages and challenges, SAFT2010, Barcelona, Spain, ,September 19-21, 2010

Zahid, Adeel, Stenby, E.H., Shapiro, A. 2010: "Improved Oil Recovery in Chalk: Wettability Alteration or Something Else?" (Oral presentation), SPE EUROPEC/EAGE Annual Conference and Exhibition, Barcelona, Spain. Full conference paper publ. in proceedings/book SPE 131300.

Zahid, Adeel, Stenby, E.H., Shapiro, A. 2010: "Advanced Waterflooding in Carbonate Reservoirs" (Poster presentation), 11th International Symposium on Evaluation of Wettability and Its Effect on Oil Recovery, 2010, University of Calgary, Alberta, Canada.

Zhang, X. 2010: "Upscaling of Waterflooding in Porous Media" (Oral presentation), 12th European Conference on the Mathematics of Oil Recovery, Oxford, Britain, 6 – 9 September, 2010. Proceedings.

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Yan, W. and Stenby, E.H. 2010: " The Influence of **CO_2** Solubility in Brine on Simulation of **CO_2** Injection into Water Flooded Reservoir and **CO_2** WAG" (Oral presentation), SPE EUROPEC/EAGE Annual Conference and Exhibition, Barcelona, Spain, 14-17 June 2010, Paper SPE 131094.

Yan, W. and Stenby, E.H. 2010: "PVT Modeling of Reservoir Fluids using PC-SAFT EoS and Soave-BWR EOS" (Oral presentation), 12th International Conference on Properties and Phase Equilibria for Product and Process Design, Suzhou, China, 16-21 May 2010.

Master Thesis 2010

Hosea Nguh Akam
"Effect of Pore Fluid on Velocity of Elastic Waves in Chalk"

Gry Andrup-Henriksen
"The crustal structure of the Eirik Ridge south off Greenland derived from forward and inverse modeling of wide-angle reflection and refraction seismic data"

Camilla Berg
"Flash Calculations for Thermal Recovery Simulations"

Michael Frost
"Measurement and Modeling of Phase Equilibrium of Oil-MEG-Water Mixtures"

Stefan Jansen
"Parameter Investigation for Subsurface Tomography with Refraction Seismic Data"

Anders Møllegaard Knage-Rasmussen
"Measurement and Modelling of Hydrocarbon Dew Points for Synthetic and Real Natural Gases"

Johanne Kuusela
"Heat Capacity Measurements of Amine-Water Solutions used for Post Combustion Carbon Dioxide Capture Applications"

Alba Caviedes Nozal
"Extraction and Crystallization of Nutritional Salts from Biomass Fly Ash"

Roelof Bjarke Pedersen
"Relative Permeability Study for Carbon Dioxide WAG"

Charlotte Elisée Eugénie Rey
"Assessment of Wells Production Profiles for Shale Gas"

Jóhanna Rasmussen
"A seismic refraction/reflection study along the FOERBAS96.01 profile
south-east of the Fraoe Islands"

Tim Rørstrøm
"Modelling of Aromatic Acids with the CPA Equation of State"

Daniel Steen Haase Sørensen
"Studies of the Influence of Enzymes on the Physical Properties of Crude Oils"

Morten Kanne Sørensen
"Acoustic Properties of Fluid Saturated Rocks"

Fie Wilbek
"Development of a Kinetic Model for the MTG Process"

Publications 2010

"Refrigeration Plants Using Carbon Dioxide as Refrigerant: Measuring and Modelling the Solubility and Diffusion of Carbon Dioxide in Polymers used as Sealing Materials"
Nicolas von Solms, and Jakob Kristensen
(International Journal of Refrigeration, 33 (2010) 19-25) SEP 0718

"Review and Recommended Thermodynamic Properties of $FeCO_3$
Philip L. Fosbøl, Kaj Thomsen, and Erling H. Stenby
(Corrosion Engineering, Science and Technology, 45(2) (2010) 115-135) SEP 0734

"Inhibition of Methane Hydrate Formation by Ice-Structuring Proteins"
Lars Jensen, Hans Ramløv, Kaj Thomsen, and Nicolas von Solms
(Ind. Eng. Chem. Res. 49 (2010) 1486-1492)
SEP 0907

A Stochastic Theory for Deep Bed Filtration Accounting for Dispersion and Size Distributions"
A.A. Shapiro, and P. G. Bedrikovetsky
(Physica A, 389 (2010) 2473-2494) SEP 0909

"Phase Equilibria Modeling of Methanol-Containing Systems with the CPA and PC-SAFT Equations of State"
Peter Chr. V. Tybjerg, Georgios M. Kontogeorgis, Michael L. Michelsen, and Erling H. Stenby
(Fluid Phase Equilibria, 288(1-2) (2010) 128-138) SEP 0913

"Preparation and Structural Characterisation of Novel and Versatile Amphiphilic Octenyl Succinic Anhydride-Modified Hyaluronic Acid Derivatives"
Corinne Eenschooten, Fanny Guillaumie, Georgios M. Kontogeorgis, Erling H. Stenby, Khadija Schwach-Abdellaoui
(Carbohydrate Polymers, 79 (2010) 597-605) SEP 0914

"Modeling of Phase Equilibria with CPA using the homomorph approach"
Martin P. Breil, Ioannis Tsivintzelis, and Georgios M. Kontogeorgis
(Fluid Phase Equilibria xx (2010) xxx-xxx (in press))
SEP 0916

"Modeling Phase Equilibria for Acid Gas Mixtures using the CPA Equation of State. Part I. Mixtures with H_2S"
Ioannis Tsivintzelis, Georgios M. Kontogeorgis, Michael L. Michelsen, and Erling H. Stenby
(AIChE Journal, 56(11) (2010) 2965-2982) SEP 0920

"Absorber Model for CO_2 Capture by Monoethanolamine"
Leila Faramarzi, Georgios M. Kontogeorgis, Michael L. Michelsen, Kaj Thomsen, and Erling H. Stenby
(Industrial and Engineering Chemistry Research, 49(8) (2010) 3751-3759) SEP 0921

"Chilled Ammonia Process for CO_2 Capture"
Victor Darde, Kaj Thomsen, Willy J.M. van Well, and Erling H. Stenby
(International Journal of Greenhouse Gas Control, 4(2) (2010) 131-136) SEP 0928

"1D Simulations for Microbial Enhanced Oil Recovery with Metabolite Partitioning"
Sidsel M. Nielsen, Alexander A. Shapiro, Michael L. Michelsen, and Erling H. Stenby
(Transport in Porous Media, 2010, 85, 785-802) SEP 0929

"Vapor-Liquid Equilibrium Measurements and Modeling of the Propyl Mercaptan + Methane + Water System"
Javeed A. Awan, Kaj Thomsen, Christophe Coquelet, Philip L. Fosbøl, and Dominique Richon
(Journal of Chemical Engineering Data, 55, (2010) 842-846) CERE 1001

"Biot´s Coefficient as an Indicator of Strength and Porosity Reduction: Calcareous Sediments from Kerguelen Plateau"
Mohammad Monzurul Alam, Mai Kristine Borre, Ida Lykke Fabricius, Kathrine Hedegaard, Birte Røgen, Zakir Hossain, Anette Susanne Krogsbøll
(Journal of Petroleum Science and Engineering, 70 (2010) 282-297) CERE 1002

"Use of Monomer Fraction Data in the Parametrization of Association Theories"

Georgios M. Kontogeorgis, Ioannis Tsivintzelis, Nicolas von Solms, Andreas Grenner, David Bøgh, Michael Frost, Anders Knage-Rasmussen, and Ioannis G. Economou
(Fluid Phase Equilibria, 296(2) (2010) 219-229) CERE 1003

"Improved Oil Recovery in Chalk: Wettability Alteration or Something Else?
Adeel Zahid, Erling H. Stenby, and Alexander A. Shapiro
(SPE 131300, prepared for presented at the SPE EUROPEC/EAGE Annual Conference and Exhibition held in Barcelona, Spain, 14-17 June, 2010) CERE 1004

"Comparison of Activity Coefficient Models for Electrolyte Systems"
Yi Lin, Antoon ten Kate, Miranda Mooijer, Javier Delgado, Philip Loldrup Fosbøl, and Kaj Thomsen
(AIChE Journal, 56(5) (2010) 1334-1352) CERE 1005

"Evaluation of the CO2 Behavior in Binary Mixtures with Alkanes, Alcohols, Acids and Esters Using the Cubic-Plus-Association Equation of State"
Mariana B. Oliveira, António José Queimada, Isabel M. Marrucho, Georgios M. Kontogeorgis, and João A.P. Coutinho
(Journal of Supercritical Fluids (in press)) CERE 1006

"Upscaling of Two-Phase Immiscible Flows in Communicating Stratified Reservoirs"
Xuan Zhang, Alexander Shapiro, and Erling H. Stenby
(Submitted to Transport in Porous Media) CERE 1007

"Modeling Non-Fickian Transport and Hyperexponential Deposition for Deep Bed Filtration"
Hao Yuan, and Alexander A. Shapiro
(Chemical Engineering Journal, 162 (2010) 974-988) CERE 1008

"In-Situ Phase Identification and Saturation Determination in Carbon Dioxide Flooding of Water Flooded Chalk Using X-ray Computed Tomography"
Ben Niu, Wei Yan, Alexander A. Shapiro, and Erling H. Stenby
(SPE 129760 - paper presented at the 17th SPE Improved Oil Recovery Symposium, Oklahoma, USA, April, 2010) CERE 1009

"Coupling Miscible Flow and Geochemistry for Carbon Dioxide Flooding into North Sea Chalk Reservoir"
Ben Niu, Wei Yan, Alexander A. Shapiro, and Erling H. Stenby
(Paper presented at COMSOL conference 2009, Milan, Italy, October 2009) CERE 1010

"Phase Identification and Saturation Determination in Carbon Dioxide Flooding of Water Flooded Chalk Using X-Ray Computed Tomography"
Ben Niu, Wei Yan, Alexander A. Shapiro, and Erling H. Stenby
(Paper presented at the International Symposium of the Society of Core Analysts, Noordwijk aan Zee, The Netherlands, September, 2009) CERE 1011

"Microbial Enhanced Oil Recovery: 3D Simulation with Gravity Effects"
S. M. Nielsen, K. Jessen, A. A. Shapiro, M. L. Michelsen, and E. H. Stenby
(SPE 131048, presented at the SPE EUROPEC/EAGE Annual Conference and Exhibition held in Barcelona, Spain, 14-17 June, 2010) CERE 1012

"Compositional Simulation of In-Situ Combustion EOR: A Study of Process Characteristics"
Priyanka Jain, Erling H. Stenby, and Nicolas von Solms
(SPE 129869, presented at the 2010 SPE Improved Oil Recovery Symposium , Tulsa, Oklahoma, USA, 24-28 April, 2010) CERE 1013

"Calculation of Liquid Water-Hydrate-Methane Vapor Phase Equilibria from Molecular"
Lars Jensen, Kaj Thomsen, Nicolas von Solms, Scott Wierzchowski, Matthew R. Walsh, Carolyn A. Koh, E. Dendy Sloan, David T. Wu, and Amadeu K. Sum
(J. Phys. Chem. B, 114, (2010) 5775-5782) CERE 1014

"Towards Predictive Association Theories"
Georgios M. Kontogeorgis, Ioannis Tsivintzelis, Michael L. Michelsen, and Erling H. Stenby
(Submitted to Fluid Phase Equilibria) CERE 1015

"Elastic Moduli of Dry and Water- Saturated Carbonates - Effect of Depositional Texture, Porosity, and Permeability"
Ida L. Fabricius, Gregor T. Bächle, and Gregor P. Eberli
(Geophysics, 75(3) (2010) N65-N78) CERE 1016

"Industrial Requirements for Thermodynamics and Transport Properties"
Eric Hendriks, Georgios M. Kontogeorgis, Ralf Dohrn, Jean-Charles de Hemptinne, Ioannis G. Economou, Ljudmila Fele Zilnik, and Velisa Vesovic
(Industrial and Engineering Chemistry Research, 49(22) (2010) 11131-11141) CERE 1017

"Analysis and Application of GCPlus Models for Property Prediction of Organic Chemical Systems"
Azizul Azri Mustaffa, Georgios M. Kontogeorgis, and Rafiqul Gani
(Fluid Phase Equilibria (in press)) CERE 1018

"Equations of State: From the Ideas of van der Waals to Association Theories"
Georgios M. Kontogeorgis, and Ioannis G. Economou
(Journal of Supercritical Fluids, 55 (2010) 421-437) CERE 1019

"High-Pressure Fluid-Phase Equilibria: Experimental Methods and Systems Investigated (2000-2004)"
Ralf Dohrn, Stephanie Peper, and José M.S. Fonseca
(Fluid Phase Equilibria, 288 (2010) 1-54) CERE 1020

"An Explanation of the Selective Plating of Laser Machined Surfaces using Surface Tension Components"
Yang Zhang, Georgios M. Kontogeorgis, and Hans Nørgaard Hansen
(Accepted by Journal of Colloid and Interface Science) CERE 1021

"Phase Equilibria of Mixtures Containing Organic Sulfur Species (OSS) and Water/Hydrocarbons: VLE Measurements and Modeling Using the Cubic-Plus-Association Equation of State"
Javeed A. Awan, Ioannis Tsivintzelis, Martin P. Breil, Christophe Coquelet, Dominique Richon, and Georgios M. Kontogeorgis
(Industrial & Engineering Chemistry Research (in press)) CERE 1022

"Experimental Determination and Modeling of the Phase Behavior for the Selective Oxidation of Benzyl Alcohol in Supercritical CO_2"
Ioannis Tsivintzelis, Matthias Josef Beier, Jan-Dierk Grunwaldt, Alfons Baiker, and Georgios M. Kontogeorgis
(Accepted by Fluid Phase Equilibria) CERE 1023

"Mutual Solubility of MEG, Water and Reservoir Fluid: Experimental Measurements and Modeling Using the CPA Equation of State"
Muhammad Riaz, Georgios M. Kontogeorgis, Erling H. Stenby, Wei Yan, Toril Haugum, Kjersti O. Christensen, Even Solbraa, and Torbjørn V. Løkken
(Fluid Phase Equilibria, (2010) DOI: 10.1016/j.fluid.2010.10.006) CERE 1024

"Partition Coefficients of Organic Molecules in Squalane and Water/Ethanol Mixtures by Molecular Dynamics Simulations"
Rasmus Lundsgaard, Georgios M. Kontogeorgis, and Ioannis G. Economou
(Submitted to Journal of Chemical Theory and Computation" CERE 1025

"Design of a Eutectic Freeze Crystallization Process for Multicomponent Waste Water Stream"
A.E. Lewis, J. Nathoo, K. Thomsen, H.J. Kramer, C.J. Witkamp, S.T. Reddy, and D.G. Randall
(Chemical Engineering Research and Design, 88 (2010) 1290-1296) CERE 1026

"Application of Association Models to Mixtures Containing Alkanolamines"
Ane S. Avlund, Daniel K. Eriksen, Georgios M. Kontogeorgis, and Michael L. Michelsen
(Submitted to Fluid Phase Equilibria) CERE 1027

"Modelling of the Thermodynamics of the Acetic Acid-Water Mixture using the CPA Equation of State"
Martin P. Breil, Georgios M. Kontogeorgis, Paul K. Behrens, and Michael L. Michelsen
(Submitted to Industrial & Engineering Chemistry Research) CERE 1028

"Comparing Ignitability for In Situ Burning of Oil Spills for an Asphaltenic, a Waxy and a Light Crude Oil as a Function of Weathering Conditions under Arctic Conditions
J. Fritt-Rasmussen, P.J. Brandvik, A. Villumsen, and E.H. Stenby
(Submitted to Cold Region Science and Technology) CERE 1029

"Composition of In Situ Burn Residue as a Function of Weathering Conditions
J. Fritt-Rasmussen, B.E. Ascanius, P.J. Brandvik, A. Villumsen, and E.H. Stenby
(Submitted to Marine Pollution Bulletin) CERE 1030

"Modeling Phase Equilibria for Acid Gas Mixtures using the CPA Equation of State. Part II. Binary Mixtures with CO_2"
Ioannis Tsivintzelis, Georgios M. Kontogeorgis, Michael L. Michelsen, and Erling H. Stenby
(Submitted to Fluid Phase Equilibria) CERE 1031

"Solid-liquid Equilibria for Binary and Ternary Systems with the Cubic-Plus-Association (CPA) Equations of State"
André Fettouhi, and Kaj Thomsen
(Fluid Phase Equilibria, 293 (2010) 121-129) CERE 1032

"Biot Critical Frequency Applied to Description of Failure and Yield of Highly Porous Chalk with Differenc pore Fluids"
Katrine Alling Andreassen, and Ida Lykke Fabricius
(Geophysics, 75(6) (2010) E205-E213) CERE 1033

"Rock Physics Model of Glauonititc Greensand from the North Sea"
Z. Hossain, T. Mukerji, J. Dvorkin, and I.L. Fabricius
(Stanford Rockphysics & Borehole Geophysics Project Annual Report 121, B1-1-B1-21) CERE 1034

"Biot Critical Frequency Applied as Common Friction Factor for Chalk with Different Pore Fluids and Temperatures"
K.A. Andreassen, and I.L. Fabricius
(Presented at the 44th US Rock Mechanics Symposium and 5th U.S. Canada Rock Mechanics Symposium, Salt Lake City, UT, June 2010, ARMA, American Rock Mechanics Association (2010) 453) CERE 1035

"Water Weakening of Chalk Explaied from a Fluid-Solid Friction Factor"
K.A. Andreassen, and I.L. Fabricius
(Rock Mechanics in the Nordic Countries, (2010) 26-35) CERE 1036

"Geostatistical Inference using Crosshole Ground-Penetrating Radar"
Majken C. Looms, Thomas M. Hansen, Knud S. Cordua, Lars Nielsen, Karsten H. Jensen, and Andrew Binley
(Geophysics, 75(6) (2010) J29-J41, DOI: 10.1190/1.3496001) CERE 1037

"Kriging Interpolation in Seismic Attribut Space Applied to the South Arne Field, North Sea"
T.M. Hansen, K. Mosegaard, and C.R. Schioett
(Geophysics, 75(6) (2010) P31-P41, DOI: 10.1190/1.3494280) CERE 1038

"A Mathematical Model for Non-monotonic Deposition Profiles in Deep Bed Filtration Systems"
Hao Yuan, and Alexander Shapiro
(E-published in journal: Chemical Engineering Journal (ISSN: 1385-8947) (DOI: 10.1016/j.cej.2010.10.036) (2010) ELSEVIER) CERE 1039

"Densification and Grain Growth during Early-stage Sintering of Ce0.9Gd0.101.95-δ in Reducing Atmosphere"
Zeming He, Hao Yuan, Julie Glasscock, Christodoulos Chatzichristodoulou, John Phair, Andreas Kaiser, Severine Ramousse
(Acta Materialia, 58(11) (2010) 3860-3866 (ISSN: 1359-6454) (DOI: 10.1016/j.actamat.2010.03.046), Pergamon) CERE 1040

"Uncertainty and Sensitivity Analysis of Filtration Models for Non-Fickian Transport and Hyperexponential Deposition"
Yuan Hao, Gürkan Sin
(Submitted to Chemical Engineering Journal) CERE 1041

"Inhibition of Structure I and II Gas Hydrates using Synthetic and Biological Kinetic Inhibitors"
Lars Jensen, Nicolas von Solms, and Kaj Thomsen
(Energy & Fuels 2010 (in press)) CERE 1042

"Sampling Informative/Complex a Priori Probability Distributions using Gibbs Sampling Assisted by Sequential Simulation"
T.M. Hansen, K. Mosegaard, and K.S. Cordua
(Presented at the 14th International Conference of the International Association for Mathematical Geosciences 29. August - 2. September 2010, Budapest, Hungary, Proceedings, 8 pp in IAMG Extended Abstract) CERE 1043

"Kriging in High Dimensional Attribute Space using Principal Component Analysis"
K. Lange, T.M. Hansen, J.L. Fernández-Martínez, J. Frydendall, and K. Mosegaard
(The 14th International Conference of the International Association for Mathematical Geosciences 29. August - 2. September 2010, Budapest, Hungary, Proceedings 10 pp in IAMG Extended Abstract) CERE 1044

"Nonlinear AVO inversion using Geostatistical a Priori Information"
K.S. Cordua, T.M. Hansen, K. Mosegaard
(The 14th International Conference of the International Association for Mathematical Geosciences 29 August - 2 September 2010, Budapest, Hungary, Proceedings, 12 pp in IAMG Extended Abstract) CERE 1045

"Monte Carlo Full Waveform Inversion of Tomographic Crosshole Data using Complex Geostatiscical a Priori Information"
Knud S. Cordua, Thomas M. Hansen, and Klaus Mosegaard
(SEG International Exposition and 80th Annual Meeting, Denver, Colorado, USA, October 2010, SEG Expanded Abstracts, 2010) CERE 1046

"Measurement and Modeling of CO2 Solubility in NaC1 Brine and CO_2-Saturated NaC1 Brine Density"
W. Yan, S.L. Huang, and E.H. Stenby
(Submitted to International Journal of Greenhouse Gas Control) CERE 1047

"Modeling of Carbon Dioxide Absorption by Aqueous Ammonia Solutions Using the Extended UNIQUAC Model"
Victor Darde, Willy J. van Well, Erling H. Stenby, and Kaj Thomsen
(Ind. Eng. Chem. Res., 49 (2010) 12663-12674(24) (CERE 1048)

"Thermodynamic Models for Industrial Applications: From Classical and Advanced Mixing Rules to Association Theories"
Georgios M. Kontogeorgis & Georgios Folas
(Wiley, January 2010, ISBN: 978-0-470-69726-9)