

Annual Report 2009





Technical University of Denmark

# Contents



We Welcome... consortium.

> Novel Gas Hydrate Inhibitors Proteins from bark beetle, meal worm and Arctic fish species are more efficient than traditional hydrate inhibitors.



To Optimize Recovery Through new mathematical tools geophysical changes in an oil and gas reservoir can be monitored during exploitation.

Chalk - not a Dusty Subject at all How much oil one can expect to recover from a field situated in chalk depends on a number of physical properties of the chalk.

-3

6

A Safe PVC Plasticiser Plasticisers that are safe to human health are in high demand in the food packaging industry primarily to replace phthalates.

**Regenerative Fuel Cells** Fuel cells can level out fluctuations in output from wind turbines, photovoltaic systems and other renewable energy sources.

18

12

## **CERE is an Expansion of IVC-SEP**

CERE Director Erling Stenby introduces the new research centre.

Sinopec Corp as a new member of the research centre's industry

By 2050 carbon capture and storage (CCS) is projected to be the world's largest single source of carbon dioxide emission reductions.

## Gearing up for Difficult Discoveries

The world still has many hidden oil and gas fields. To find them requires sophisticated mathematical tools.

## Highlights from an Extraordinary Year

The most exciting development in 2009 for IVC-SEP was of course the upgrading of the centre to CERE.

# CERE is an Expansion of IVC-SEP

Through our new name, the energy related activities of the research centre become more visible. Still, the strong focus on thermodynamics of the former IVC-SEP remains the centre's backbone.

to the 2009 Annual Report of the Engineering Research Center for Phase Equilibria and Separation Processes (IVC-SEP) - a report which also marks the transformation of the centre into the Center for Energy Resources Engineering (CERE). For quite some time we have desired to increase the visibility of the energy related activities of the centre. Hence our new name.

However, the change of name is more than just symbolic. Supported by a strategic decision by DTU's top management, we have been able to strengthen existing strongholds of IVC-SEP while also including new research fields relevant to our core activities. As an example, the inclusion of geophysical and geological Faculty members function as a natural extension of the research already done under IVC-SEP 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. They will become associated CERE Faculty members.

#### A global challenge

Despite general consensus on the need to develop a renewable energy future, all realistic estimates point to oil, gas and coal as strongly needed on the medium term. According to International Energy Agency forecasts, oil demand will increase from 85 mb/d (million barrels per day) in 2006 to 99 mb/d in 2015 and 116 mb/d in 2030. Some 42 per cent of this increase is projected to come from China and India alone. This rising trend in demand cannot easily be

met by new discoveries or increased exploitation of existing fields. Thus, the global society face a huge challenge in meeting the demand until more sustainable sources are matured and able to take over. CE-RE will play a part in meeting this challenge – both through our research and through our education.

The new structure allows us to act as a one-stop "shopping" for energy resources engineering research at DTU. A company may present us with a problem t is with great enthusiasm that I welcome you and we will identify the relevant academic resources at DTU and set up the relevant group - often multidisciplinary - for the specific task.

#### Responsible transition

The term Energy Resources Engineering does obviously not refer to oil and gas exclusively. CCS is also a very active research area for CERE and we are ready to engage in research into other sources of energy, while careful not to duplicate efforts already ongoing in other institutions and departments. For example we see geothermal energy as one field where our longstanding engagement within thermodynamics combined with our new academic resources within geology and geophysics may prosper.

At CERE we see ourselves as a part of responsible transition to a sustainable energy future.

Finally I would like to stress that the change of 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 be able to strengthen research related to chemical industry processes, food manufacturing and others - not least through the establishment of a new position as chair in thermodynamics

All in all we are proud of the enhanced academic possibilities we have been given. We will do all we can to put them to use over the coming years.

> Professor Erling Stenby, Director of CERE



Erling Stenby Director of CERE, professor ehs@cere.dtu.dk

"Dear Members of the Consortium"

Excerpt from joint letter by Lars Pallesen, DTU Rector, and Erling Stenby, CERE Director, to the CERE Consortium, November 2009.

"The Technical University of Denmark (DTU) has decided to expand and promote the Engineering Research Center for Phase Equilibria and Separation Processes (IVC-SEP) to a stronger and more clearly defined research centre within the university. This is done in recognition of the performance of the IVC-SEP and due to the importance of the areas where the centre has reached an internationally leading position. We acknowledge that the Consortium - currently with 29 member companies - has played a key role in the centre's 30 year history. The consortium

DTU has decided to use IVC-SEP as the backbone of a new initiative namely an Energy Resources Engineering Center to ensure that DTU as a whole can act and perform efficiently within this important area. The new centre will include all of the current activities within IVC-SEP and several new activities at other departments of DTU. In the future you can expect to find the same flexibility in the centre's activity as today but we have decided to emphasize the energy

related activities in the name in order to increase the visibility of these activities. In Energy Resources Engineering we include oil and gas (production, transport, refining, GTL, a.o.), carbon capture and storage, and geothermal energy exploitation, but we do not limit the scope of the centre to this. We want to underline that the generic research within applied thermodynamics will be brought forward and strengthened and the same is true for the non-energy related research such as mineral extraction, material science, food science, and chemical product development. We also want to increase our efforts within colloid and surface chemistry. Furthermore the Faculty members joining the centre at other departments at DTU will bring in new research topics.

We look very much forward to continue our fruitful collaboration with the Consortium,"

# The Consortium - our Strongest Asset

CERE is supported by public means from several sources, e.g. The Danish Research Council for Technology and Production Sciences and The Nordic Energy Research Programme. Furthermore the Center is supported by grants from several private companies. The strongest asset of CERE is the industrial Consortium. Approximately 20-25 companies are members, the exact number changes due to the dynamics of

the industry's mergers and acquisitions. The member companies closely follow the activities of the Center. This ensures that CERE activities are relevant in relation to the topical problems and limitations in existing knowledge within applied thermodynamics. This ongoing external control of quality and inspiration assist in maintaining the CERE research at the highest international level.

4

Lars Pallesen, DTU Rector Erling Stenby, CERE Director

## CERE Consortium:

- Statoil
- Maersk Oil
- Gaz de France
- ConocoPhillips
- Haldor Topsøe
- BP
- Linde
- Eni
- Total
- DONG Energy
- Shell
- INEOS
- GASSCO
- OMV
- Chevron
- Kommunekemi
- Petrobras
- SOM
- RWF
- Akzo Nobel
- IFP
- Schlumberger
- ExxonMobil
- Vattenfall
- Welltec
- Saudi Aramco
- Sasol
- Sinopec
- Llovd's Register ODŠ



## We welcome Sinopec

China Petroleum & Chemical Corporation – or Sinopec Corp – is one of the largest integrated energy and chemical companies in China.

The scope of its business mainly covers oil and gas exploration and production, extraction, pipeline transmission and marketing; oil refining; production, marketing, storage and transportation of

petrochemicals, chemical fibres, chemical fertilizers and other chemical products.

Sinopec is China's largest producer and supplier of refined oil products (including gasoline, diesel and jet fuel) and major petrochemical products. It is also China's second largest crude oil producer.

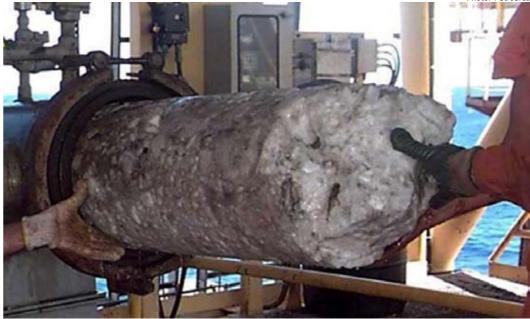
# Proteins from Nature May Replace Synthetic Gas Hydrate Inhibitors

Large quantities of gas hydrate inhibitors, primarily methanol and glycol, are needed presently to secure recovery under cold and high-pressure conditions. Research at CERE suggests that proteins found in organisms like bark beetle, meal worm and Arctic fish species can do the job far more efficiently.

This is a novel approach to an old problem in oil and gas recovery. And when we first realized the potential, it was a completely unexpected approach - even to ourselves."

Nicolas von Solms, CERE faculty member, speaks with enthusiasm of results obtained by PhD Student Lars Jensen under his supervision.

Gas hydrates are substances resembling snow or ice consisting of water and light hydrocarbons. Under certain conditions they will precipitate in pipes and production gear. This again may lead to production stops implying major economical losses.



A combination of low temperature, high pressure and presence of water is known to provide ideal conditions for hydrate formation. Unfortunately those are exactly the conditions you have to face when recovering at Northern locations or deep water. Presently large quantities of inhibitors, primarily methanol and ethylene glycol, are utilized. As much as 40 % concentration of gas hydrate inhibitors may be seen in the fluid phase under recovery and transportation of oil and gas at Northern locations.

#### Slows the pace of reactions

Methanol and glycol both work by lowering the temperature point at which hydrate formation starts pretty much like the same substances are used in vehicles to lower the freezing point of water. A few years ago the idea came up of replacing the large quantities of these inhibitors with polymers. Rather than lowering the temperature point of hydrate formation, the polymers act as a negative catalyst which inhibits key chemical processes involved. This is called a kinetic gas hydrate inhibitor.

"Actually a kinetic inhibitor does not really prevent hydrate formation - it just slows down the pace of reactions. But for practical purposes the job will be

Photo: Petrobra

Gas hydrates are substances resembling snow or ice consisting of water and light hydrocarbons. Under certain conditions they will precipitate in pipes and production gear during oil and gas exploitation. This may again lead to production stops implying major economical losses.

Statoil is an integrated technology-based international energy company primarily focused on upstream oil and gas operations. Headquartered in Norway, the company has more than 30 years of experience from the Norwegian continental shelf, pioneering complex offshore projects under the toughest conditions. Statoil has about 30,000 employees in 40 countries. The company is the world's largest operator in waters more than 100 meters deep. Production averages more than 1.7 million barrels of oil equivalent per day. Proven reserves are more than six billion barrels of oil equivalent.



Certain naturally occurring proteins have been shown to be extremely efficient as gas hydrate inhibitors. Especially efficient are proteins from bark beetle. Under certain conditions the CERE team couldn't see any hydrate formation for as

much as 24 hours.

not present all along the production line. Once the gas stream reaches the platform, pressure will be lower and temperature higher. So if you can prevent the formation of hydrates for long enough – a few hours to a day, you have succeeded," von Solms explains.

done, since the conditions for hydrate formation are

The really good news is that kinetic inhibitors are efficient in much smaller quantities compared to traditional inhibitors. Unlike methanol and glycol, which have to be present in large concentrations in the entire liquid phase the kinetic inhibitors work in small quantities due to their role as catalysts. Less that one per cent of kinetic polymers are needed compared to traditional inhibitors.

#### Inspired by Arctic fish

Commercial products are already available and used at some locations. However, these polymers are not biodegradable and are therefore not allowed everywhere. For instance they are banned from use in the North Sea due to environmental concerns.

The researchers at CERE (then IVC-SEP) started out by categorizing the processes involved when polymers act as kinetic gas hydrate inhibitors. Next step was to look for other substances that would be able to do the trick but was also biodegradable. Various substances were tried without being really promising, until the team began looking for substances occurring in nature.

"We already knew that proteins found in various Arctic and deep sea fish species were candidates as these substances are a key to survival under cold and relatively high pressure conditions. While the freezing of water and hydrate formation are not exactly the same processes there are a number of chemical similarities, so one would assume that the same substances that help fish survive in cold water may also inhibit hydrate formation. In fact, the commercially available polymers were inspired by deep sea fish proteins from the outset," Nicolas von Solms says.

From that point on surprises started to come.

"Our research confirmed that fish proteins worked, but as we moved on to proteins found in insects we saw them to be considerably more efficient. Proteins from meal worms are really good, and proteins from bark beetle are even better. Under certain conditions we couldn't see any hydrate formation for as much as 24 hours."

#### Statoil: High relevance

Statoil is the world's largest operator of deepwater fields. The company also undertakes a large proportion of its activities in the high North, meaning an increased exposure to hydrate formation conditions.

"Statoil has for decades had a close cooperation with CERE and its leading scientists. This work of Lars Jensen and his supervisor Nicolas von Solms is yet another example of the creativity and world leading competence on thermodynamics found at the centre," comments Per Gerhard Grini, Chief Researcher on Upstream Process and Flow Assurance Technology, Statoil R & D Centre.

"Our exploration after oil and gas has a strong focus towards the Arctic environments, and hydrate formation is therefore one of our toughest challenges. Therefore, low dosage hydrate inhibitors with more environment friendly properties are of high relevance to us," Per Gerhard Grini ads.

#### Costs need to come down

The best proteins proved ten times more efficient compared to commercially available polymers – which again makes them 1,000 times more efficient compared to traditional inhibitors. A naïve assumption would be that this ratio should allow proteins to easily enter the market.

"This is not the case as these proteins presently are way too expensive. But the good news is that once an interest is created, production can be optimized in several ways leading to a remarkably lower price," Nicolas von Solms comments.

"First of all these proteins could be produced in yeast or other micro organisms and secondly once a company with expertise in this kind of production comes in it will soon be able to produce much more efficiently. Thirdly, by improving our understanding of the chemical processes involved we expect to refine the use of the proteins so that even smaller amounts can suffice."

Besides a better basic understanding of the chemistry, CERE researchers face quite a few tasks before the development of actual commercial products can begin.

"Until now we have focused on demonstrating the effect in purified water. This is of course not what you have in the liquid phase in real oil and gas recovery. We will now begin to demonstrate the effect in salty water and in water containing various types of particles."

> Polymers that act as kinetic hydrate inhibitors are already commercially available. Some of these polymers were inspired by proteins found in deep sea fish the same substances that help fish survive in cold water may also inhibit hydrate formation.

## As our exploration after oil and gas

has a strong focus towards the Arctic, hydrate formation is one of our toughest challenges. Therefore, low dosage hydrate inhibitors with more environment friendly properties are of high relevance to us.

Per Gerhard Grini, Chief Researcher on Upstream Process and Flow Assurance Technology, Statoil R & D Centre. Photo: Bigstockphoto



# **Cleaner** Coal - A Necessary Part of **Climate Protection**

Over the coming decades a large part of the world's total reduction in annual greenhouse gas emissions needs to come from carbon capture and storage (CCS). CCS will continue to be a high priority to CERE.

hile the much highlighted UN conference on climate change, COP15, in December 2009 did not provide a clear picture of how the global community will tackle climate change, the challenge remains the same. By the end of this century a number of renewable resources are likely to be developed to a stage where they can contribute to global energy supply on a massive scale, but until then we still need fossil fuels. Thus, we need to learn to exploit fossil fuels in ways that contribute less to global warming.

Reducing carbon dioxide emissions from coal fired power plants through carbon capture and storage (CCS) is one of the solutions with the highest potential for CO2 reduction over the coming decades. CCS describes the chain of processes whereby carbon dioxide is sequestered from the power plant process before or after combustion, compressed, and then stored in geological formations. CCS in coal-fired power plants

GHG Emissions Reductions: Solutions for 2050

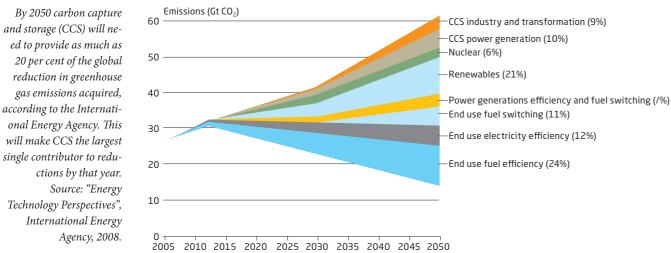
will provide a crucial bridging solution, enabling substantial reductions in carbon dioxide emissions from coal fired power plants.

#### One fifth of the solution

According to the International Energy Agency almost 20 per cent of the total greenhouse gas emissions reductions we need to achieve in 2050 needs to come from CCS. IEA projections show that energy sector CO<sub>2</sub> emissions will increase by 13 per cent by 2050 in the absence of new policies or supply constrains as a result of increased fossil fuel usage.

IEA's latest Energy Technology Perspectives state that "the only technology available to mitigate greenhouse gas emissions from large-scale fossil fuel usage is carbon dioxide capture and storage". Without CCS "overall costs to halve emissions by 2050 (will) rise by 70 per cent."

How development of CCS technologies will be financed and put to practical use is still unclear. One idea is to include CCS in the climate protection mechanisms endorsed by the UN-backed Clean Development Mechanism (CDM). Here, industrialised nations are given carbon credits as they support clean energy projects in third world countries. This is seen as a cost-effective way of keeping down emissions - as reductions in developed world countries are generally more expensive to achieve. The first discussions on including CCS in the CDM were



taken during the COP15 conference but no decision was taken.

Ahead of the UN conference in Copenhagen several politicians voiced their support for CCS at a conference of the Carbon Sequestration Leadership Forum in London.

"We agree there is no possible solution (...) without CCS as part of it. The world will use coal, oil and gas in the future. We want to raise this debate and get more countries involved," Terje Riis-Johansen, Norwegian Energy Minister, told AFP.

His British colleague, Ed Miliband, said: "We need technology cooperation for know-how and capacitybuilding, and a financing agreement (...) which can drive CCS forward in developing countries."

#### OECD countries must lead

According to the International Energy Agency between 2.4 trillion and 3.4 trillion US dollars is needed for CCS investments in the years leading up to 2050. This is about 6 percent of the total investment necessary to halve the world's carbon emissions compared to the 2005 level.

"OECD countries must lead in the first decade but the technology must very quickly expand to the developing world, where the vast bulk of emissions growth will take place," Nobuo Tanaka, Executive Director of IEA, said in a press release.

Presently only demonstration projects are operational, and none of them including the entire circle from carbon capture to storage. All projects are in industrialized countries with Norway, Germany, UK and USA as leaders. However, South Africa is about to join the club. At the conference in London, Energy Minister Dipuo Peters said her country intends to test carbon injection by 2016 and have a demonstration plant capable of storing 100,000 tonnes of carbon dioxide annually ready by 2020.

#### CCS at CERE

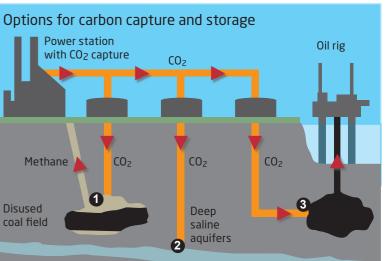
For a number of years CERE has undertaken research within CCS. Several capture technologies are investigated in cooperation with members of the centre's industry consortium, including major research projects in cooperation with Vattenfall and DONG Energy. "I am pleased to say that with the inclusion of new academic staff within geophysics and geology to the centre, our ability to provide "the full package" within CCS is further strengthened. We are strongly committed to becoming one of the internationally leading CCS centres," says CERE director Erling Stenby.

Methane

Disused coal field

Source: World Coal Institute, BBC

gas emissions by 2050 will rise by 70 per cent The International Energy Agency



1 CO<sub>2</sub> pumped into disused coal fields displaces methane which can be used as fuel

2 CO<sub>2</sub> can be pumped into and stored safely in deep saline aquifers

3 CO<sub>2</sub> pumped into oil fields helps maintain pressure, making extraction easier

## CCS according to the International **Energy Agency**

Without carbon **Z** capture and storage overall costs to halve greenhouse

CCS is an important part of the lowest cost greenhouse gas mitigation portfolio; without CCS, overall costs to halve emissions by 2050 rise by 70 per cent. This roadmap envisions 100 projects globally by 2020 and over 3,000 projects in 2050.

This roadmap requires a total investment of over USD 6 trillion between 2010-50; this is about 6 per cent of the overall investment needed to achieve a 50 per cent reduction in greenhouse gas emissions in 2050.

The developed world must lead in the next decade, but CCS technology must spread rapidly to the rest of the world. This will require expanded international collaboration and financing for CCS demonstration in developing countries at an average annual level of USD 2-4 billion between 2010-20.

CCS is more than a strategy for "clean coal". CCS technology must be adopted by biomass and gas power plants, in the fuel transformation and gas processing sectors, and in emissions-intensive sectors like cement, iron & steel and chemicals manufacturing.

The milestones in this roadmap will only be achievable via expanded international collaboration. New efforts to provide developing country knowledge/ technology transfer are needed. Industry sectors with a global reach should also expand their CCS collaborative efforts.

Highlights from "Energy Technology Perspectives", International Energy Agency, 2008.

As part of ongoing

research and development

efforts, Vattenfall initia-

ted a project on CCS in

2001. The goal of the pro-

ject is to develop commer-

cial concepts for CCS at

power plants between

2015 and 2020.

#### Photo: Vattenfal

operation during 2010.

In Denmark, Vattenfall is undertaking investigations on CCS at The Nordjylland Power Station (Nordjyllandsværket) in Aalborg. The investigations include assessments of deep geological structures in Northern Jutland. Initial assessments have indicated the geology to be well suited for long-term storage of CO<sub>2</sub>.

Thermal Power.

sides of CCS. This is due to the fact that the core of both disciplines is thermodynamics which is also CERE's academic core. As soon as you move into practical engineering, capture and storage becomes very different - which is also why it is normally organized separately - but

for CERE it is obviously an asset to be able to include both. This is quite unique."

# The Race to Become the Chosen Capture Technique

Some techniques are already proven technically efficient. However, CO<sub>2</sub> capture is still at an early stage. Several candidates compete to become the solution of choice.

Up to 90 percent of carbon dioxide produced in the combustion process at coal fired power plants can be captured with the technologies presently at hand. However, costs are still too high for these technologies to be ready for use. Several technologies compete to become the one that gets the job done - while also being the most cost-effective approach.

The research at CERE mainly focuses on technologies which may be used at both existing and new steam power plants - meaning scrubbing technologies that capture CO<sub>2</sub> after combustion. DONG Energy and Vattenfall jointly sponsor a project on Post-Combustion Capture of CO<sub>2</sub> from Fossil Fuel Power Plants. The aim is to develop design tools for CO<sub>2</sub> absorption units using aqueous alkanolamines as absorbents. The joint sponsorship covers half of the funding, while The Danish Research Councils cover the other half.

In 2009, CERE concluded the creation of software which enables plant operators to not only simulate CO<sub>2</sub> capture but also integrate this simulation into the normal plant operation software. Source code

has been transferred from the centre to the energy companies involved.

Besides amine solution techniques other ongoing CERE projects study ionic fluids and protein based capture techniques.

#### First carbon lean electricity by 2015

Four years ago DONG Energy installed a pilot plant in Esbjerg. After a normal combustion process the flue gas is led to an additional process facility. CE-RE takes part in the academic support base behind the project.

In the facility the CO<sub>2</sub> content of the flue gas is exposed to an amine solution (amines are organic compounds derived from ammonia, NH<sup>3</sup>). The mixture is then boiled resulting in the release of  $CO_2$ . Finally the CO<sub>2</sub> is compressed to make it ready for storage.

As part of ongoing research and development efforts, Vattenfall initiated a project on CCS in 2001. The goal of the project is to develop commercial concepts for CCS at power plants between 2015 and 2020. Vattenfall operates a number of test rigs, EU projects and joint efforts at different pilot and research stations around the world.

Vattenfall has built a 30 MW pilot plant for carbon dioxide capture at the lignite-fired power

latest years.

plant at Schwarze Pumpe, Germany. The plant was inaugurated in 2008. Next step will be a full-scale demonstration plant at Jänschwalde in Germany. The project is planned to deliver CO<sub>2</sub> lean electricity to the grid in 2015. Through Nuon, Vattenfall is building a pilot plant at the Willem Alexander power plant in Buggenum, Netherlands. It is planned to be in

#### Vattenfall: CCS will grow globally

"One can hardly doubt that CCS will constitute a key element in turning power production climate neutral. We have to realize that between the energy system of today and that of the future we will have a transition period in which coal is included. At Vattenfall we view CCS at a global scale. It may happen that we scale down activities in one country but if you take a broader view things keep going up. This area will definitely grow," says Hakon Mosbech, Nordic head of engineering at Vattenfall's division

Vattenfall has worked with CERE on a number of technology projects on carbon capture over the

"One special feature of the research centre is its ability to deal with both the capture and the storage side of CCS. Here at Vattenfall we are also active both within capture and within storage. Yet, these activities are organized under different divisions which is a general picture both in the industry and in the academic world," says Hakon Mosbech and continues:

"It is interesting that CERE is able to address both

### Vattenfall

Vattenfall is Europe's fifth largest generator of electricity and the largest generator of heat. The company currently has operations in Denmark, Finland, Germany, United Kingdom, Poland, Netherlands and Sweden. Vattenfall is active at all stages of the electricity value chain - generation, transmission, distribution and sales. Vattenfall also generates, distributes and sells heat, and conducts energy trading and lignite mining. The parent company, Vattenfall AB, is wholly owned by the Swedish state.

As soon as you **Z** move into practical engineering, capture and storage becomes very different - which is also why it is normally organized separately - but for CERE it is obviously an asset to be able to include both. This is guite unique.

Hakon Mosbech, Nordic head of engineering at Vattenfall's division **Thermal Power.** 

# To Optimize Recovery

As injection of water and other means of EOR (Enhanced Oil Recovery) are applied, rather than waiting to see what will become the final result one should monitor the geophysical implications along the way to adjust the process in due time.

The world's oil fields presently have an expected average recovery rate of less than 50 per cent. The potential economic and energy supply benefits if one can raise that rate are vast.

"Even a marginal increase in the rate of recovery from an oil field will easily justify the effort we are putting into this area of research," says Professor, geophysicist Klaus Mosegaard, who newly has become member of the CERE faculty.

Having worked within energy resources during earlier stages of his career, Klaus Mosegaard comes from a position at the Niels Bohr Institute of the University of Copenhagen where he mainly did academic research related to the interior of the Earth and the Moon. However, especially one project conducted over the latest years has proved most relevant to the oil and gas industry.

"In many structures knowledge of pore sizes and permeability are the key to optimize recovery rates. If you have data from seismic measurements that give you a picture of the geological structure and also measurements showing the flow of oil, gas and water through the field you are able to say a lot about permeability properties. However, each of these two sets of data will typically be so large that the capacity of even the largest scientific computers is challenged. Joining them would thus seem practically impossible. Our idea was to develop a method to break down these vast complexes of calculations into minor parts in order to allow computers to handle them," Klaus Mosegaard explains, adding:

"Our ambition was merely to provide rough estimates, but once the method was in place, it proved to be surprisingly accurate."

This success was one of the reasons why Mosegaard's group joined CERE by the beginning of 2010. "Naturally we wanted to develop the methodology further in order to actually raise recovery rates in specific oil fields. This was in obvious accordance with the ambitions of the IVC-SEP, now CERE, and the merger was straight forward. All modesty put aside I think it is fair to say that the centre is contributing at a high level. You might think that we're just a tiny centre in one small country, but if you look at the academic partners and industry consortium behind CERE, you'd think again. All the leading companies in the industry and most top universities internationally are associated. Every player you'd want to cooperate with is here. Therefore what we're doing is far more than just a local effort," Mosegaard says.

The methodology has a dual perspective. Firstly, if one knows the properties of an oil field in great detail, recovery can be planned more accurately from the outset. Secondly, data obtained during recovery may be utilized to adjust one's recovery strategy along the way.

"As production starts and oil, gas and injected water begin to flow, new seismic measurements may provide a much clearer picture of the underground "pipe system" of that particular structure. Which areas have higher or lower permeability? These data may be assessed on a yearly or even monthly basis in order to adjust e.g. the water injection strategy and potentially raise the recovery rate."

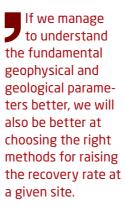
#### More than history matching

DONG Energy is a co-sponsor of CERE's geophysical research.

"Quite naturally, a large amount of R & D in the oil and gas industry is aimed at enhancing the recovery rate in already existing fields. A lot of research in MEOR (Microbial Enhanced Oil Recovery) and  $CO_2$  EOR, polymers etc. is taking place. Another, more practical angle is to establish where exactly oil is left behind," comments Morten Gjetting Stage, R&D Manager, DONG E&P, Petroleum Engineering Department.

This could also be a significant role for geophysics, Morten Gjetting Stage feels:

"Until recently we have tried to understand the performance of our reservoirs by optimization of a number of flow parameters in our reservoir simulation models. This has been based on the assumption that our fundamental geological model was correct. Some of the projects undertaken by CERE are not only focussed on modifying the flow parameters to make the model match the production history – but also includes fundamental geophysical and geological parameters. If we manage to do this better, we will also be better at choosing the right methods for raising the recovery rate at a given site." When the geophysical properties of an oil field are known in great detail, recovery can be planned more accurately from the outset. Secondly, data obtained during recovery may be utilized to adjust one's recovery strategy along the way.



Morten Gjetting Stage, R&D Manager, DONG Energy Photo: DONG Energy



# If Chalk Sounds Like a Dusty Subject to You - Think Again

The North Sea is one region where oil fields are situated in chalk. How much oil one can expect to find in a given field and to what extent it may be recovered depends highly on a number of physical properties of the chalk including its permeability. CERE has upgraded its geological expertise.

Research at CERE into permeability studies of geological structures is supported by the Danish Research Council for Technology and Production (FTP) and by DONG Energy.

Scanning electron micrographs of chalk of Maastri chtian age. (A) Partially or fully broken coccoliths from Stevns chalk with a porosity of 50%. The thin rods are modern organic remains. (B) Recrystallized chalk from Tor Formation of South Arne field with a porosity of 30%. Images were recorded by Morten Hjuler.

A successful defence of a doctorial thesis on Applysical properties of chalk may sound like an event of interest to a limited number of academic colleagues only. However, as quite a large number of oil fields are situated in chalk - for example most fields in the Danish North Sea - the subject of Associate Professor, and now Dr. Techn., Ida Lykke Fabricius' thesis is also of genuine interest to the oil and gas industry.

Maintaining her status as a member of the DTU Institute of Environment and Resources faculty, Ida Lykke Fabricius has now become a full member of CERE - allowing the centre to complement the knowhow within oil and gas processing and recovery of its progenitor, the IVC-SEP, with geological expertise.

"I already had a great deal of cooperation with the IVC-SEP faculty and with members of the centre's industry consortium, so I see it as a natural step to become a full member of CERE. Also, cooperation with industry gives you access to a wealth of data that would otherwise have been beyond your reach as a scientist," Ida Lykke Fabricius says.

#### Take internal pressure into account

Chalk is a sedimentary rock with highly variable properties. Especially the chalk's permeability is of interest to oil and gas exploration.

A crude assumption would be that the deeper the chalk is situated, the lower its permeability would be due to the pressure from above. However, this is a far too simplistic picture, Ida Lykke Fabricius explains:

"The pressure from above is to some extent counteracted by the internal pressure caused by the chalks content of oil and water. You need to subtract this effect. For instance, not so many decades ago geologists thought one would never be able to find oil in North Sea chalk as the pressure from water and rock above would have squeezed out any oil long time ago. They had forgotten to take internal pressure into account. And as we now know, oil is indeed present!"

Another simplistic assumption would be that the older the chalk, the lower its permeability due to so

called cementation, meaning chemical reactions where chemical substances are shifted around via dissolution in the water. This would gradually lessen the pore size of the chalk.

#### Impurities determine permeability

Ida Lykke Fabricius uses a can with sweet drops as a model to prove her point.

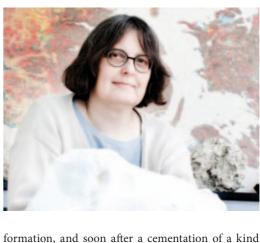
"Over time the drops will tend to bond together. This can be compared to cementation in chalk. However, while the grains stick more and more together, the pore volume does not change and the size of each pore may even grow so that the overall permeability increases. This type of cementation also contributes to strengthen the structure."

Still, cementation is not just one process but many because the composition of chalk is highly variable. For instance, depending on ocean temperature and other variables at the time when the chalk was sedimented the content of various fossils will vary. Warm surface temperatures at the time tend to form a chalk rich in calcareous nanofossils while cold water favours silicious nanofossils. These variations in composition lead to different patterns in cementation - and some of these may actually make the pore sizes smaller leading again to a steady decrease in permeability over time.

"As a rule of thumb a very pure chalk will preserve its permeability to relatively high burial and it may even improve over time, while chalk with a high content of clay and silica tends to gradually drop in permeability," Ida Lykke Fabricius states.

#### "A super reservoir"

The present permeability is of great significance to actual recovery - how much oil can be squeezed out and how should one go about it? - but also the permeability history of a site is important. Ideally the chalk would have had high permeability at the time of oil

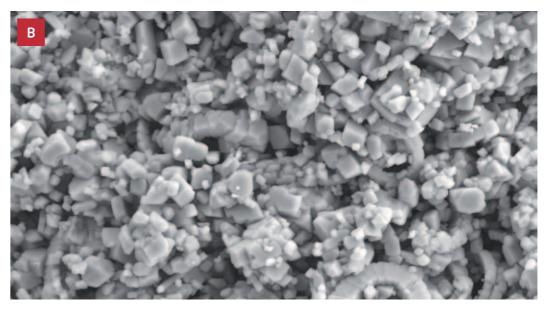


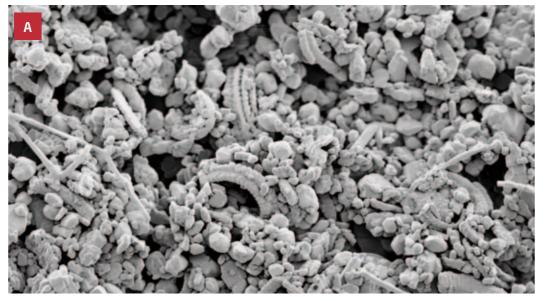
the oil inside the reservoir.

community:

It should be noted that papers on chalk is of interest to other sectors than oil and gas recovery. Chalk is used as a raw material for cement, as a means of controlling acidity in soil and neutralizing acid gasses generated in power plants, as filler in paper and plastic and as white pigment. Also a number of built structures - for instance the Øresund Fixed Link between Denmark and Sweden - are constructed on chalk.

field of geothermal heating.





that drastically decreased permeability took place in the border zone to the surrounding rock - trapping

"That would give you a super reservoir," Ida Lykke Fabricius says with a smile that reveals her awareness of the interest in her research outside the scientific

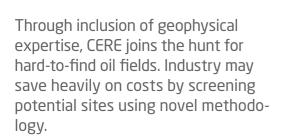
"Even though my primary interest has been academic for the last many years, I have always enjoyed cooperation with industry. Actually I began my career working four years at Maersk Oil."

Finally, the geological expertise of Ida Lykke Fabricius and her colleagues may be required in a number of future CERE projects for instance in the

As many oil fields are situated in chalk – for example most fields in the Danish North Sea – the subject of Associate Professor, Dr. Techn., Ida Lvkke Fabricius' research is of genuine interest to the oil and gas industry.

Maersk Oil has **Z** through the years always had a fruitful research collaboration with the Institute of Environment and Resources at DTU. With Ida Lykke Fabricius becoming a full member of CERE we look forward to expand this collaboration. Henrik Tirsgaard, Chief Geologist, Maersk Oil, **Corporate Techno**logy & Projects

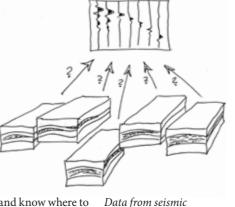
# The Era of Easy Discovery is over



honestly believe this may help industry avoiding some costly mistakes."

Geophysicist Klaus Mosegaard, Professor at CERE, does not have a magic formula for finding well hidden oil reserves. Still, his research group is able to assist the search by quantifying the likelihood of a number of competing hypotheses that might explain a given pattern in seismic measurement results.

"The era where one could point to apparent ano-



malies in the geological structures and know where to drill, is over. All these easy discoveries have been made. Still you have a number of potential fields out there. For instance you may have oil trapped inside an area *fields do tend to show* with large porosity and permeability which is capped by areas with low permeability. To find these types of discrete fields - or just to increase the likelihood of finding them – we have to stretch our data from seismic measurements to the limit," Klaus Mosegaard says.

Oil reserves that are hidden in areas with high porosity, but with similar basic geological composition as their impermeable surroundings are known as stratigraphic oil fields.

"Until you actually start drilling all you have is seismic data. Data from measurements done on areas with stratigraphic fields do tend to show certain patterns, but typically these results could have come from other structures also. What my group does is basically to list

measurements on areas with stratigraphic oil certain patterns, but typically these results could have come from other structures also. The ambition of CERE's geophysical group is to list the entire family of possibly explanations to a given set of data, and then to apply a probability for each of them to be the accurate one. Illustration Klaus Mosegaard

# "One Stop Shopping for Industry"

From now on  $\mathbf{Z}$  we will be able to simply state what our problem is and CERE will then coordinate which academic resources should go into a project. We see this as a major advantage.

> **Morten Gjetting** Stage, **R&D Manager**, **DONG Energy**

DONG Energy, sponsor of the research at CERE related to discovery of stratigraphic oil fields, welcomes the new organisation in Denmark of research related to oil and gas recovery.

**O** nly by extracting more information from already available data can one hope to discover new oil and gas reservoirs in areas where major fields have already been exploited. And to achieve that we need to find improved mathematical methods of processing our seismic data - so that reservoirs of a smaller physical scale may be identified," says Morten Gjetting Stage, R&D Manager, DONG E&P, Petroleum Engineering Department. The company funds the research by Professor Klaus Mosegaard's group related to discovery of stratigraphic oil fields.

"The size of these reservoirs is just one problem - they may also have smaller relief and thus be hard to distinguish from other packages of sedimentary layers," says Morten Gjetting Stage. For DONG Energy the creation of CERE opens new perspectives, he feels:

"We welcome that oil and gas related research is now unified in one organisation. This enables an industry partner like our selves to do one stop shopping. Most problems we face go beyond borderlines between academic disciplines. Instead of acting as agents that try to encourage four or five different research groups to cooperate, from now on we will be able to simply state what our problem

the entire family of possibly explanations to a given set of data, and then to apply a probability for each of them to be the accurate one."

#### Crunching thousands of equations

Moving from seismic measurements to actual drilling, costs accelerate.

"The economic implications of unsuccessful discovery operations are large, and it is only natural that many companies within the industry have been hesitant when they are faced with a family of possible explanations to data - with only one of them including an oil field. However, as existing fields are exploited the need to find new fields is becoming ever more acute. If we can apply a probability to the various competing hypotheses and thus help industry to avoid mistakes, we can really save large economic resources."

Smilingly, the Professor admits this to be easier said than done.

"We have to tackle vast complexes of calculations. I still remember how proud I was when, back in the 7th grade of primary school I managed to solve my first set of dual equations with two unknown variables. Today the complexes we solve may contain thousands of equations and thousands of unknowns."

#### Inspired by Moon science

Klaus Mosegaard started off working three years at Maersk Oil, but his career has been academic since.

is and CERE will then coordinate which academic resources should go into a project. We see this as a major advantage."

#### Larger research projects can be launched

Through CERE, research related to oil and gas discovery and recovery may receive a boost, the DONG Energy R & D Manager hopes:

"In view of the importance to society of oil and gas recovery I think it is fair to say that the area is in low priority at the Danish universities. The universities may have launched quite a large number of vessels, but some of them never reach their final destination, while those that do are sometimes too small to really make an impact. Joining the forces in CERE will increase the likeliness of projects reaching their targets and being large enough to make a difference," says Morten Gjetting Stage.

"Also, I am optimistic that the new organization will strengthen the research overall. For instance the centre will be better positioned to build strong partnerships with other universities primarily abroad. Further, the structure should encourage the academic society to develop this area - both within basic and applied penhagen.

"For instance I have contributed to recent science on the Moon's interior. In cooperation with NASA scientists we were allowed to make use of old seismic data from the landings. Using modern methodology one can derive quite a lot more from these data compared to what was possible back in the 1970'ies. This is of course very academic compared to energy discovery at Earth, but from a scientific angle the work you need to do is not that much different."

Klaus Mosegaards interest in solving tasks involving huge calculations explains why his office is not found in the same building as CERE's core activities at The Technical University of Denmark (DTU), but at DTU Informatics.

"While still a full CERE faculty member, I get access to cutting edge developments within scientific computing by physically sitting here with the top number crunchers of DTU. This gives me a unique role to bridge the expertise within energy research and the contacts to industry of CERE with scientific computing."

research which may in turn contribute to knowledge building in both industry and the university." Stronger education

Finally, Morten Gjetting Stage expects the educational aspect to be strengthened:

"We consider candidates to be an output just as important as the results from the centre's research itself. They are crucial to the future of the industry. As things stand today we at DONG Energy are often impelled to recruit new employees internationally. This has both advantages and downsides."

an example:

"We have more than ten nationalities represented in a staff of 30. Employees who graduated abroad tend to be more mobile compared to employees that graduated in Denmark. They will typically stay here some years and move on. They bring us a wealth of new ideas that we really appreciate. However, we also need to have a number of employees that stay for a long time in order for us to maintain continuity. When we employ a candidate who has graduated in Denmark, we increase the likelihood of that."

He has had several periods of leave working for engineering companies, but until he joined CE-RE at the beginning of 2010, he was employed at the Niels Bohr Institute at the University of Co-

Klaus Mosegaard

The era where **Z** one could point to apparent anomalies in the geological structures and know where to drill, is over. To find stratigraphic fields we have to stretch our data from seismic measurements to the limit.

> Klaus Mosegaard, Professor, CERE

The R & D Manager takes his own department as

DONG Energy is one of Northern Europe's leading energy groups. Its business is based on procuring, producing, distributing, trading and selling energy and related products in Northern Europe. DONG Energy has interests in 75 gas and oil exploration licenses throughout Denmark, Norway, UK, the Faroe Islands, and Greenland

# Validation of Migration Modelling of PVC Plasticiser into Food Products

Plasticisers that are fully biodegradable and safe to human health are in high demand in the food packaging industry primarily to replace phthalates. CERE research shows that months of laboratory tests to validate the safety of plasticisers can be replaced by computer modelling.

ests that normally take up to several months and require the efforts of skilled lab technicians can be replaced by the first five per cent of data when coupled with computer based estimations.

"Regulation - especially EU legislation - has a high focus on migration of substances from packaging into food. In this regard we benefit from a model developed at CERE with our cooperation," says Bjarne Nielsen, Senior Application Manager, Plastics Tech, Danisco.

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, marketed as Soft-N-Safe, is a fully acetylated glycerol monoester with a 10 percent content of fully acetylated glycerol monostearate. It is 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.

> As much as 40-60 volume percent of most PVC products is plasticiser – as without plasticiser PVC would be very rigid and brittle. Hence plasticisers that are safe to human health are in high demand - i.e. for PVC used in food

"Depending on which type of food you are packaging you are looking at very different solvents - ranging all the way from wet food to very fatty. The model estimates migration of a given substance into various solvents. It is valuable to be able to estimate the migration instead of needing to undertake extensive measurements every time a new situation is at hand. And the model developed at CERE has been shown to accurately reflect real events," says Bjarne Nielsen.

#### Ready for industry to use

For many applications PVC has been the first choice of plastic during several decades mainly due to its solidness and high durability. However, within recent years PVC manufacturers have seen setbacks because of distrust in the plasticisers used, mainly phthalates. As much as 40-60 volume percent of most PVC products is plasticiser - as without plasticiser PVC would be very rigid and brittle. Hence alternative plasticisers like Soft-N-Safe are in demand.

"Some biodegradable plasticisers have been shown to be safe to human health and environment through extensive testing. What we have done is to demonstrate a valid and much faster way to evaluate new, chemically related products," explains Ph.D. student Rasmus Lundsgaard, CERE.

He stresses that the new method has been approved by Danish and EU food safety authorities and is thus ready to be put to use by industry.

Danisco and CERE has undertaken a joint research project on safety issues related to Soft-N-Safe and similar products.

"Any tiny change a manufacturer would make in the formulation or the way a product is synthesised requires a new approval if the product is to be used in relation to food. However, we have shown that one does not need to undertake a full migration survey if the new product is chemically closely related to another product that has already been extensively surveyed," Lundsgaard explains further.

#### A barrier in the surface

Modelling migration of plasticiser from the packaging into one of four food stimulants given by the EU legislation is a key element for the approval of a new food product in the European market.

the ability to accurately estimate the migration for any given migrant in the polymer is the project's core output. For Danisco the project holds perspectives that reach beyond the Soft-N-Safe product. "Actually we are considering the method to become a part of our product development," reveals Danisco's Bjarne Nielsen. "For some additives you may actually desire migration to the surface of the packaging. We can use the model to calculate which substances will be most suited in a given situation. The choice of possible solutions is very wide so if you are able to narrow down the number of promising options through modelling you may save significant amounts of time. One may so to speak take a short cut in one's laboratory work."





Lundsgaard.

"When PVC is used for food packaging a certain amount of plasticiser migration into the food is inevitable. However, the migration is not in all cases as large as one might think," says Rasmus

This is mainly due to two factors. Firstly, because the solubility of Soft-N-Safe and similar plasticisers is very low in hydrophilic products. The solubility is often lower than the systematic migration limit set up by the EU.

"Secondly, we have observed for very hydrophobic solvents that the overall migration was lower than calculated at first. It is proposed through the knowledge from our migration models that once a certain amount of plasticiser from the outer layer of the PVC has migrated into the surroundings, the emptied outer layer will then act as a barrier against further migration," according to Lundsgaard.

#### New applications for the method

Migration is not just one-way from PVC into food. "From the consumer's point of view only the migration of plasticisers from the PVC into the food is important, but the migration of fatty food content into the PVC will also have some effect on the PVC and hence the overall plasticiser migration into the food," says Rasmus Lundsgaard, adding that

In 2005 Danisco launched an alternative plasticiser for use in PVC for food packaging. The product, marketed as Soft-N-Safe, is produced from castor oil. Extensive testing including animal testing has demonstrated absolutely no harmful effects from the product.

We can use the model to calculate which substances will be most suited in a given situation. The choice of possible solutions is very wide so if you are able to narrow down the number of promising options through modelling you may save significant amounts of time.

Bjarne Nielsen, Senior Application Manager, Plastics Tech, Danisco

# Regenerative Fuel Cells to Support Renewable Energy

Lloyds Register ODS sees regenerative fuel cells, which are able to level out fluctuations in output from wind turbines, photovoltaic systems and other renewable energy sources as a key element in future energy systems.

One of the drawbacks of renewable energy sources is that their availability is not always coincident with real world electrical loads. For example, a photovoltaic system installed at a single residence will not provide any power for that residence at night or in the early morning. Similarly, the output from wind turbines is highly variable and fluctuations will not coincide with consumption patterns. A potential solution to these types of problems is the regenerative fuel cell.

While a fuel cell normally acts as a small scale power station producing electricity from oxygen (typically from the air) and hydrogen (typically from natural gas), a regenerative cell is able to do the opposite. In a period of excess power production from i.e. photovoltaic systems or wind turbines, the regenerative cell will recharge its batteries consisting of aqueous electrolyte solutions and thereby store energy. During a later period with low power production and peak consumption the charged electrolyte solutions may be utilized for power production either in the same (regenerative) fuel cell or in a fuel cell optimized for power production.

#### Modelling the cell's thermodynamics

"The public's desire to have less polluting, cleaner energy will continue to drive growth in energy sources such as wind, solar and biomass. While having the advantage of being renewable and clean these energy sources are all variable. So, we need some kind of energy storage to flatten out these patterns of wild spikes and low production that you would otherwise get. In fact, the lack of energy storage solutions is currently holding back a lot of investments in renewable energy. Regenerative fuel cells are one promising type of solution," says The lack of energy storage solutions is currently holding back a lot of investments in renewable energy. Regenerative fuel cells are one promising type of solution.

Sean Cuthbert, Principal Consultant Lloyds Register ODS Sean Cuthbert, Principal Consultant, Lloyds Register ODS.

Through joint support from the company itself and the Danish Council for Technology and Innovation (RTI), Sean Cuthbert will work as an Industrial PhD student at CERE for the next three years. He will be supervised by associate professor Kaj Thomsen. The core of the project will be to develop thermodynamic and multi-scale / multi-physic models that can be generally applied to evaluate regenerative fuel cell designs. Upon completion performance of the models is to be verified by an independent academic faculty abroad.

"The thermodynamic behaviour of a regenerative fuel cell is complex and not well understood. Currently there is a need to develop a vigorous, reliable model that can be used to optimize these cells," says Sean Cuthbert.

#### Increasing demand for consultancy

Using the future model as a screening tool, Lloyds Register ODS will take feed-in parameters from new designs for regenerative fuel cells developed by its clients into the model.

"The results should help us to asses whether the cell will perform as expected – and could the performance possibly be improved further? We will also address issues like the safety of the public, including a Life Cycle Assessment (LCA) which is always a key question to us," Sean Cuthbert explains.

"We are confident that such a model can be developed building on theoretical work at CERE and using the centre's Extended UNIQUAC thermodynamic model for electrolyte systems."

Still, the company does not see the model as the only outcome of the project, Cuthbert notes:

"Just as important will be the expertise regarding regenerative fuel cells that I will acquire during the project and will disseminate within the company. We expect that an increasing number of our clients will demand consultancy specific to energy storage technology. In order to review their designs we need to be abreast and preferably slightly ahead of technology developments in this field. At Lloyds Register ODS we are convinced that regenerative fuel cells will become a key element in future energy systems."

#### Photo: DONG Energy

Lloyds Register ODS is a global engineering firm specializing in advanced simulation technology for the design and analysis of complex structures and systems. The company provides solutions to structural, materials and environmental problems using advanced engineering simulation software tools. Lloyds Register ODS employs more than 150 consultants based at offices in Denmark, Sweden, Norway, England, France, China and Canada.

# Highlights from an **Extraordinary Year**



Director of CERE,

ehs@cere.dtu.dk

professor

The most exciting development of the year was of course the upgrading of the center to CERE (Center for Energy Resources Engineering) - and the following range of interesting new possibilities.

n 2009 we have seen a strengthening of the core activities in the center, which will remain highly prioritized within the new structure. We are thus proud to present the highlights from a well-established yet dynamic center in progress.

In this IVC-SEP/CERE Annual Report for 2009 we are presenting samples of our ongoing and recently completed research activities. While it cannot do justice to all the hard work done and excellent results obtained by the more than 40 coworkers in the center, at the very least I hope you will be able to see if we work in areas of interest to you.

We are always keen on providing the best possibilities for our PhD students to strengthen their scientific skills and support their development. Therefore, we are also pleased to announce that José Fonseca, PhD student at the center, received the ESAT 09 award for Best Student Paper. The paper concerned the testing of a new high-pressure, low-temperature apparatus for measuring three-phase equilibria in certain inhibitor systems. José Fonseca project is under the supervision of Nicolas von Solms.

The annual Discussion Meeting of IVC-SEP took place for the 30th time from 10-12 June in Comwell, Holte. Again we enjoyed the excellent attendance of our member companies, and the scientific discussions and interactions between colleagues and external participants were as always very fruitful indeed. We will of course continue this significant yearly event for the Center under the new and upgraded CERE structure. Please see our home page for details.

#### The Consortium

The IVC-SEP, now CERE Consortium continues its positive development. During 2009 we have welcomed Sinopec from China. We are proud of the variety of important companies involved in the ener-

gy industrial and chemical sectors represented. With the formation of CERE, the ambition is not only to maintain the high relevance and quality of our research for our member companies - but to extend it even further, both with regard to scope and excellence.

We do not exclusively cooperate with the Consortium but enjoy an open dialogue with many external parties. Where mutual interests are present the possibility for organizing a shared project often finds its way, and we are happy to offer the know-how, research experience and innovative skills established through our many years of working in the front line of the scientific fields we cover.

#### Major ongoing projects

Below are listed the major ongoing projects including the level of man power working at IVC-SEP/ CERE in 2009 directly on each project:

• Advanced Water Flooding for enhanced Oil recovery 2009 - 2011. 1 PhD project added to the ADORE project as DONG Energy joined as sponsor. The ADORE project is originally funded by the Danish

Council for Independent Research and Maersk Oil. · CompSim is a joint project with University of Bergen regarding improvements in compositional reservoir simulation. Two post docs are funded by ENI. • CHIGP II 2007-2012 (originally an acronym for "Chemicals in Gas Processing". Over the years many other applications have been added, but we have kept the name). This highly successful JIP co-ordinated by Georgios Kontogeorgis has in its second phase been running since 1 January 2007. The sponsors are Maersk Oil, DONG Energy, Statoil, Gassco, BP and Total. The development of the CPA EOS takes place in this project and the continuously updated CAPE Open version of CPA is one of the primary deliverables of the JIP. Another is an Aspen Plus User model of the CPA EOS. The project is further strengthened by a post doc grant from the Danish Agency for Science, Technology and Innovation and an additional PhD grant from Statoil. • The last major theme to mention is "CO2 Capture and Storage". In addition to our EOR activities we now have activity within the following postcombustion processes: alkanol amines, chilled ammonia, amino acid salt solutions, and ionic liquids. All of these processes



The images display moments captured during Oilsim Course, IVC-SEP Summer School, DM Poster Session, PhD course and other significant 2009 events.

## ...Highlights from an Extraordinary Year

present tough challenges when it comes to simulation of the actual capture process. In addition to the modeling and simulation work we are involved in the establishment of a pilot plant. We now have 6 coworkers in this area and we will expand our CCS activities during 2010.

• Also, the novel and exciting History Matching activities lead by Klaus Mosegaard and described elsewhere in the present report falls under the EOR theme. It is funded by the Danish Agency for Science, Technology and Innovation. We are looking very much forward to developing this and the above mentioned projects further in CERE in 2010 and onwards. Again we welcome collaboration and input from the member companies.

#### High and further increasing activity

With the new structure we have secured a very high level of activity in CERE for the coming year. My expectation is that it will probably increase further due to the extended possibilities within the new center structure and the currently ongoing negotiations and pending applications submitted to various funding agencies and companies.

At the end of this report you will have an overview of the manuscripts produced by the IVC-SEP coworkers during 2009. Members of the CERE Consortium can download all of these from our web site, and anyone can contact us for copies of any of the published papers, including papers from Ida Fabricius and Klaus Mosegaard. Their future publications will be included in the CERE publication list. Our website www.cere.dtu.dk also contains information about our research software, SPECS, our CAPE-OPEN tools and our extensive electrolyte database.

In June 2010 we will arrange the PhD course in "Molecular Simulation of Complex Chemical Systems with Emphasis to Practical Applications, and in August 2010 we will once again organize the Summer school on "Thermodynamic Models: Fundamentals & Computational Aspects" by Michael Michelsen.

If this status, the report or our website raises any questions please do not hesitate to contact me or any of my colleagues at CERE. We look forward to continuing the fruitful collaboration with the industrial Consortium and our academic partners.

## Ph.D. Summer School 2009

he bi-annual IVC-SEP/CERE Summer School "Petroleum Fluids. Properties of Production" took place 10 to 28 August, 2009.

In total, there were 18 participants, from IVC-SEP, from the different academic institutions, as well as from the industry.

The school gives overview over the thermodynamic of petroleum fluids, and over their flows in porous media of petroleum reservoirs. It touches such modern and industrially important subjects as fluid distribution in petroleum reservoirs; properties of gas hydrates; properties of petroleum engineering-related electrolytes; petroleum asphaltenes; enhanced oil recovery with gas and, especially, carbon dioxide injection (with a perspective of its storage and application to petroleum industry); and others. The school was very positively evaluated by its participants.

Cismondi.

North America.

time in August.



## DTU PhD course in Argentina

The course "Thermodynamic models: Fundamentals and computational aspects" has been held twice in 2009. At DTU as usual, in January, but also in Cordoba, Argentina, in later October, by invitation from our collaborator Professor Martin

The course participation (21) was, as expected, dominated by South America, but in addition to that there was also attendance from Europe as well as from

In 2010, the course will again be given at DTU, this

## **Research Funding** in IVC-SEP/CERE 2009

s a university research group our job objective Ris 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 ahead into 2010 the centre is to receive additional 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 2009 our external research funding has increased to a total budget of EUR 3.2 million. Looking external funding due to projects brought into the centre by incoming faculty members Klaus Mosegaard and Ida Lykke Fabricius.

Re	search Funding			0	
	for 2009 the main g presented in the follo		$\mathbf{\mathbf{N}}$		
Pro	ojects 2009	(kEUR)			
AD CO CC Gas Phi Ott	IGP ORE 2 EOR S s Hydrates D grants DTU her Private her Public	391 460 256 445 100 364 766 380	Ŕ		
Tot	tal external funding	3,162			5
		-			

# **Conference Contributions** and Invited Speakers 2009

#### Waheed Afzal, Oral presentation. Estimation of the Impact of Sulfur Species on Glycol Dehydration.

Afzal, Waheed; Breil, Martin Peter; Mohammadi, Amir H.; Kontogeorgis, Georgios; Richon, Dominique.

EQUIFASE 2009. Porto, Portugal, 2009 EQUIFASE 2009.

#### Ane Søgaard Avlund, Oral presentation. Intramolecular Association within the SAFT framework.

Avlund, Ane Søgaard; Kontogeorgis, Georgios; Michelsen, Michael Locht; Chapman, W.G. Therodynamics 2009, 2009 Book of abstracts: Thermodynamics 2009.

#### Ane Søgaard Avlund, Poster presentation. Intramolecular Association within the SAFT Framework.

Avlund, Ane S. Kontogeorgis, Georgios M., Michelsen, Michael L., Chapman, Walter G. Presented at: JETC10. Copenhagen, Denmark, 2009, JETC10

Victor Darde, Poster presentation.

### Aqueous Ammonia Process for CO<sub>2</sub> Capture Darde, Victor Camille Alfred; Thomsen, Kai; van Well, Willy J.M.; Stenby, Erling Halfdan. IARU Climate Congress. Copenhagen, 2009

Victor Darde, Oral presentation. Aqueous Ammonia Process for CO<sub>2</sub> Capture Darde, Victor Camille Alfred; Thomsen, Kaj; van Well, Willy J.M.; Stenby, Erling Halfdan. Risø International Energy Conference, 2009 Energy solutions for CO<sub>2</sub> emission peak and subsequent decline. Proceedings.



### Victor Darde, Oral presentation. Using Fundamental Advanced Thermodynamics to Model CO<sub>2</sub> Capture Using Aqueous Ammonia. Darde, Victor Camille Alfred; Thomsen, Kaj; van Well, Willy J.M.; Stenby, Erling Halfdan. 12th Meeting of the International Post-combustion CO<sub>2</sub> Capture Network. Regina, Canada, 2009.

### Victor Darde, Oral presentation. Using Fundamental Advanced Thermodynamics to understand a CO<sub>2</sub> Capture Process. Darde, Victor Camille Alfred; Thomsen, Kaj; van

## ...Conference Contributions and Invited Speakers 2009

Well, Willy J.M.; Stenby, Erling Halfdan. SIMS50 Conference, Skærbæk, Denmark, 2009 SIMS50.

### losé Fonseca, Poster presentation. Design, Construction and Testing of a New High-Pressure, Low-Temperature Apparatus for Measuring Three-Phase Equilibria in Hydrocarbon-Water-Hydrate Inhibitor Systems Fonseca, José; von Solms, Nicolas. 24th ESAT European Symposium on Applied Thermodynamics, Santiago de Compostela, Spain, 2009 Book of abstracts: 24th ESAT, 86. Received the ESAT-award for best poster.

### José Fonseca, Poster presentation. Modelling Phase Equilibrium in Gas Hydrate Inhibitor Systems Using Simplified PC-SAFT Fonseca, José; Swaminathan, Saravana; von Solms, Nicolas.

Presented at: 24th ESAT. Santiago de Compostela, Spain, 2009 Book of abstracts of the 24th European Symposium on Applied Thermodynamics, 184.

#### José Fonseca, Poster presentation. A New High-Pressure, Low Temperature Apparatus for the Study of Phase Equilibria through a Synthetic Method.

Fonseca, José; von Solms, Nicolas. Equifase 2009 - VIII Iberoamerican Conference on Phase Equilibria and Fluid Properties for Process Design . Algarve, Portugal, 2009 Book of abstracts: Equifase 2009, 157.

### Philip Loldrup Fosbøl, Poster presentation. Corrosion in Pipelines.

Philip L. Fosbøl, Kaj Thomsen, and Erling H. Stenby MCE Deep Water, Copenhagen, Denmark, March, 2009.

### Philip Loldrup Fosbøl, Poster presentation. Corrosion in Pipelines.

Philip L. Fosbøl, Kaj Thomsen, and Erling H. Stenby SPE meeting, DTU, Lyngby, Denmark, April, 2009.

### Philip Loldrup Fosbøl, Poster presentation. CO<sub>2</sub> capture and storage projects at IVC-SEP.

Philip L. Fosbøl SPE meeting, DTU, Lyngby, Denmark, April, 2009.

### Philip Loldrup Fosbøl, Oral presentation. The Chilled Ammonia Process (CAP) - Energy Requirements by Thermodynamic Modeling. Philip L. Fosbøl, Kaj Thomsen, and Erling H. Stenby Proceedings 24th ESAT conference, Santiago de Compostela, Spain, June, 2009.

### Philip Loldrup Fosbøl, Poster presentation. Thermodynamics of irreversible processes enhanced by mixed solvent electrolyte activity coefficient models.

Philip L. Fosbøl, Kaj Thomsen, and Erling H. Stenby Proceedings JETC10, Copenhagen, Denmark, June, 2009.

#### Philip Loldrup Fosbøl, Oral presentation.

Energy demand for CO<sub>2</sub> solvent regeneration. Philip L. Fosbøl, Kaj Thomsen, and Erling H. Stenby Proceeding Risø International Energy Conference, p. 242-252, Roskilde, Denmark, September, 2009.

#### Philip Loldrup Fosbøl, Oral presentation.

Improving Mechanistic CO<sub>2</sub> Corrosion Models . Fosbøl, Philip Loldrup; Thomsen, Kaj; Stenby, Erling Halfdan.

CORROSION 2009. Atlanta, Georgia, USA , 2009 Proceedings CORROSION/09; Paper no. 09561.

#### Philip Loldrup Fosbøl, Poster presentation. Thermodynamics of Irreversible Processes Enhanced by Mixed Solvent Electrolyte Activity

**Coefficient Models.** Denmark, 2009 JETC10

Georgios Kontogeorgis, Oral presentation. Recent Developments of the CPA equation of state for associating fluids. Kontogeorgis, Georgios; Tsivintzelis, Ioannis; Breil, Martin Peter; Tybjerg, Peter Chr. V.; Stenby, Erling Halfdan; Michelsen, Michael Locht. 24th ESAT European Symposium on Applied Thermodynamics, 2009 Book of Abstracts: 24th ESAT, 74.

Solvents.

Kontogeorgis, Georgios; Tsivintzelis, Ioannis; Economou, Ioannis. DCIS2009 Danish Colloid and Interface Symposium. University of Aarhus, Denmark , 2009 DCIS 2009 Danish Colloid and Interface Symposium.

mics Conference.



Fosbøl, Philip Loldrup; Thomsen, Kaj; Stenby, Erling Halfdan. Presented at: JETC10. Copenhagen,

### Georgios Kontogeorgis, Invited speaker. Modelling the Solubility of Pharmaceuticals in Liquid and Supercritical Pure and Mixed

#### Georgios Kontogeorgis, Invited speaker. Capabilities and Limitations of Association

Theories. Kontogeorgis, Georgios; Tihic, A.; Folas, Georgios; Tsivintzelis, Ioannis; Grenner, Andreas; von Solms, Nicolas; Constantinou, L.; Economou, Ioannis; Michelsen, Michael Locht.

JETC 10 - Joint European Thermodynamics Conference, 2009 JETC 10 Joint European Thermodyna-

## ...Conference Contributions and Invited Speakers 2009

### Georgios Kontogeorgis, Oral presentation. The Role of Monomer Fraction Data in Association Theories.

Kontogeorgis, Georgios; von Solms, Nicolas; Tsivintzelis, Ioannis; Grenner, Andreas; Bøgh, David; Frost, Michael; Knage-Rasmussen, Anders; Economou, Ioannis; Michelsen, Michael Locht.

Equifase 2009 - VIII Iberoamerican Conference on Phase Equilibria and Fluid Properties for Process Design , 2009 Book of abstracts: Equifase 2009, 32.

#### Georgios Kontogeorgis, Oral presentation. Capabilities and Limitations of Association Theories

Kontogeorgis, Georgios; Tihic, A.; Folas, Georgios; Tsivintzelis, Ioannis; Grenner, Andreas; von Solms, Nicolas; Constantinou, L.; Economou, Ioannis; Michelsen, Michael Locht.. Thermodynamics 2009. Imperial College London, UK , 2009 Book of abstracts: Thermodynamics 2009

#### Benedicte Mai Lerche, Oral presentation. CO<sub>2</sub> Capture from Flue Gas using Amino Acid Salt Solutions .

Lerche, Benedicte Mai; Stenby, Erling Halfdan; Thomsen, Kaj.

Risø International Energy Conference, 2009 Energy solutions for CO<sub>2</sub> emission peak and subsequent decline. Proceedings.

#### Rasmus Lundsgaard, Poster presentation. Modeling partition coefficients of additives in polymer/polymer and polymer/solvent systems by free energy calculations. Lundsgaard, Rasmus; Kontogeorgis, Georgios;

Economou, Ioannis. 24th ESAT European Symposium on Applied Thermodynamics . Santiago de Compostela, Spain, 2009 Book of abstracts: 24th ESAT, 234.

### Bjørn Maribo-Mogensen, Poster presentation. Modelling Separation Processes of Mixed

#### Solvent-Electrolyte Systems Using an Extended UNIQUAC User Model Implemented in ASPEN Plus.

Bjørn Maribo-Mogensen, Kaj Thomsen, and Martin P. Breil. Proceedings from 24th ESAT European Symposium on Applied Thermodynamics.

## Ben Niu, Oral presentation.

Phase Identification and Saturation **Determination in Carbon Dioxide Flooding of** Water Flooded Chalk Using X-Ray Computed Tomography.

Niu, Ben; Yan, Wei; Shapiro, Wei Yan; Stenby, Erling Halfdan.

Presented at: International Symposium of the Society of Core Analysists . Noordwijl aan Zee, The Netherlands, 2009 Proceeding from International Symposium of the Society of Core Analysists.

#### Ben Niu, Oral presentation.

Coupling Miscible Flow and Geochemistry for Carbon Dioxide Flooding into North Sea Chalk Reservoir.

Niu, Ben; Yan, Wei; Shapiro, Alexander; Stenby, Erling Halfdan.

Presented at: European COMSOL Conference 2009 . Milan, Italy, 2009 Proceeding in CD from European COMSOL Conference.

#### Sidsel M. Nielsen, Oral presentation. Mathematical Model for Microbial Enhanced Oil Recovery with Surfactant Distributed Between Phases.

Nielsen, M. Sidsel; Shapiro, A. Alexander; Michelsen, L. Michael; Stenby, H. Erling 30th IEA-EOR, Canberra, Australia, September 2009.

#### Negar Sadegh, Oral presentation. Thermodynamic Modeling of Water-Acid Gases-Alkanolamine Systems.

Sadegh, Negar; Thomsen, Kaj; Stenby, Erling Halfdan; Kontogeorgis, Georgios. Presented at the 9th AIChE Annual Meeting 2009, Nashville, TN, USA.

#### Alexander Shapiro, Oral presentation. Stochastic Modeling of Particle Migration in Porous Media Accounting for Dispersion and Size Distributions.

Shapiro, A.A.; Bedrikovetsky, P.G.; 30th IEA-EOR, Canberra, Australia, September 2009.

#### Nicolas von Solms, Poster Presentation. Modeling Gas Hydrates Using Simplified PC-SAFT.

von Solms, Nicolas; Swaminathan, Saravana; Michelsen, Michael Locht; Kontogeorgis, Georgios

24th ESAT European Symposium on Applied Thermodynamics . Santiago de Compostela, Spain, 2009 Book of abstracts: 24th ESAT, 180.

#### Nicolas von Solms, Invited speaker.

Inhibition of Gas Hydrate Formation by Low-Dosage, Environmentally Benign Inhibitors. von Solms, Nicolas; Fosbøl, L. Philip

Presented at: Equifase 2009 - VIII Iberoamerican Conference on Phase Equilibria and Fluid Properties for Process Design, 2009 Book of abstracts: Equifase 2009, 45.

#### Nicolas von Solms, Invited speaker.

Inhibition of Gas Hydrate Formation by Low-Dosage, Environmentally Benign Inhibitors. von Solms, Nicolas; Fosbøl, L. Philip Presented at: SPE meeting, DTU, Lyngby, Denmark, April 2009.

### Nicolas von Solms, Oral presentation. Experiences with CDIO in an integrated Product- and Process Design Course. von Solms, Nicolas; Vigild, E. Martin; Grunwaldt, Jan-Dierk; Kiil, Søren; Clement, H. Carsten Presented at: International CDIO Conference, Singapore, 2009.

## Erling Stenby, Invited speaker.

"PVT and Gas Injection", Invited lectures at CIPR, University of Bergen, 12-13 March 2009

#### Erling Stenby, Invited speaker.

"Petroleum Research at CERE", Invited lecture at Maersk Oil Qatar, 31 May 2009

## Erling Stenby, Invited speaker. "Phase Identification and Saturation

Determination in Carbon Dioxide Flooding of Water Flooded Chalk Using X-ray Computed Tomography",

Ben Niu, Alexander A. Shapiro, Wei Yan, and

Australia

"EOR Research at CERE", September 2009

Erling Stenby, Invited speaker. "Petroleum Research at CERE", Invited lecture at GDF-SUEZ, Paris, 10 December 2009

Thomsen, Kaj.

Solvents. Kontogeorgis, Georgios.

2009

Wei Yan, Poster presentation. Measurements and Modelling of CO<sub>2</sub> Solubility in Brine and CO<sub>2</sub>-Saturated Brine **Densities at High Pressures.** Yan, W., Huang, S. and Stenby, E.H., International Conference on Deep Saline Aquifers for Geological Storage of CO<sub>2</sub> and Energy at IFP/Rueil-Malmaison, France, May 27-29, 2009.

Wei Yan, Oral presentation. CO<sub>2</sub> Flooding Simulation. Yan, W. and Stenby, E.H. Orleans, LA, USA, October 4-7, 2009, SPE 124628

Erling H. Stenby, IEA-EOR Workshop and Symposium 2009, 21-23 September, Canberra,

## Erling Stenby, Invited speaker. Invited lecture at University of Adelaide, 25

### Kaj Thomsen, Oral presentation. Phase Equilibria in Aqueous Solutions of Fly-ash From Biomass Combustion.

24th ESAT European Symposium on Applied Thermodynamics . Santiago de Compostela, Spain, 2009 Book of abstracts: 24th ESAT, 62.

### Ioannis Tsivintzelis, Oral presentation. Modeling the Solubility of Pharmaceuticals in Liquid and Supercritical Pure and Mixed

Tsivintzelis, Ioannis; Economou, Ioannis; 24th ESAT European Symposium on Applied Thermodynamics. Santiago de Compostela,

Spain, 2009 Book of abstracts: 24th ESAT, 157.

## Ioannis Tsivintzelis, Poster presentaion. Modeling the Complex Hydrogen Bonding Behavior of Mixtures with Glycols.

Tsivintzelis, Ioannis; Kontogeorgis Georgios. Presented at: JETC10. Copenhagen, Denmark,

# The Influence of CO<sub>2</sub> Solubility in Brine on Proceedings from the 2009 SPE ATCE, New

## Master Thesis 2009

Grydgaard, Anne "Modeling of Absorption Cooling in a Process Plant"

Herslund, Peter Jørgensen and Claus Maarup Rasmussen "Effect of Environmental and Operational Conditions on Solar Evaporation Ponds"

Kaltsouni, Vasiliki "Distribution of Complex Chemicals in Oil-Water Systems"

Lorentz-Petersen, Janus "Phase Equilibria and Properties of CO<sub>2</sub>-water Mixtures"

Waseem Arshad, Muhammad "CO<sub>2</sub> Capture using lonic Liquids"

Yasin, Soniasara "Analysis of Scaling Risks in Oil and Gas Production Systems"

Yuan, Hao "Enhanced Oil Recovery"

# Publications 2009

#### SEP 0901

mental Analysis of Mixed-Solvent Electrolyte Systems"

Philip L. Fosbøl, Kaj Thomsen, and Erling H. Stenby

(Journal of Solution Chemistry, 38(1) (2009) 1)

#### SEP 0902

"Reaction Kinetics of Acetone Peroxide Formation and Structure Investigations Using Raman Spectroscopy and X-ray Diffraction"

L. Jensen, P. M. Mortensen, R. Trane, P. Harris, and R. W. Berg

(Applied Spectroscopy, 63(1) (2009) 92-97)

#### SEP 0903

"Solubility Measurements in the Mixed Solvent Electrolyte System Na2CO3-NaHCO3-Monoethylene Glycol-Water"

Philip L. Fosbøl, Kaj Thomsen, and Erling H. Stenby

(Industrial & Engineering Chemistry Research., 48 (2009) 2218-2228)

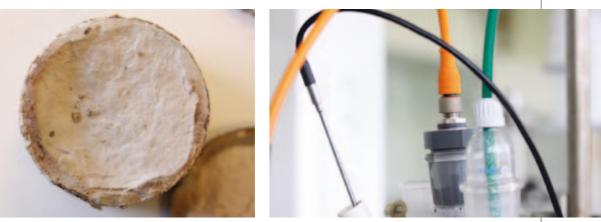
SEP 0904

"Modeling the Vapor - Liquid equilibria of Polymer - Solvent Mixtures: Emphasizing on Systems with Complex - Hydrogen Bonding Behavior"

Ioannis Tsivintzelis, and Georgios M. Kontogeorgis







109)

SEP 0905 Chloride)" (2009) 147-158)

SEP 0906 Stenby

SEP 0907 Ice-Structuring Proteins" Nicolas von Solms

SEP 0908

## "Reverse Schreinemakers Method for Experi-

(Fluid Phase Equilibria, 280(1-2) (2009) 100-

"Modeling of the Migration of Glycerol Monoester Plasticizers in Highly Plasticized Poly(vinyl

Rasmus Lundsgaard, Georgios M. Kontogeorgis, Jørgen K. Kristiansen, and Torkil F. Jensen (Journal of Vinyl and Additive Technology, 15

"Improving Mechanistic CO<sub>2</sub> Corrosion Models" Philip L. Fosbøl, Kaj Thomsen, and Erling H.

(Presented at the CORROSION 2009 . Atlanta, Georgia, USA, 2009 Proceedings CORRO-SION/09 ; Paper no. 09561)

"Inhibition of Methane Hydrate Formation by Lars Jensen, Hans Ramløv, Kaj Thomsen, and (Ind. Eng. Chem. Res. 49 (2010) 1486-1492)

"Addition of Malodorants to Lighter Gas - A Study of the Physical Properties of Mixtures" Vasu Neela, and Nicolas von Solms (Submitted to Journal of Chem. Inf. Model.)

## ...Publications 2009

#### SEP 0909

A Stochastic Theory for Deep Bed Filtration Accounting for Dispersion and Size Distributions" A. Shapiro and P. G. Bedrikovetsky (Submitte to Physica A)

#### SEP 0910

"Modeling of the Mixed Solvent Electrolyte System CO<sub>2</sub> - Na2CO3 - NaHCO3 - Monoethylene Glycol - Water Philip L. Fosbøl, Kaj Thomsen, and Erling H. Stenby

(Ind. Eng. Chem. Res. 48 (2009) 4565-4578)

#### SEP 0911

"Phase Equilibria of Mixtures Contatining Glycols and the n-Alkanes: Experimental Study of Infinite Dilution Activity Coefficients and Modeling using the Cubic-Plus-Association Equation of State" Waheed Afzal, Martin P. Breil, Pascal Théveneau, Amir H. Mohammadi, Georgios M. Kontogeorgis, and Dominique Richon (Industrial & Engineering Chemistry Research, 48(24) (2009) 11202-11210)

#### SEP 0912

"Electrodeposition of Asphaltenes. 1. Preliminary Studies on Electrodeposition from **Oil-Heptane Mixtures**"

D. S. Khvostichenko, and S. I. Andersen (Enery and Fuels, 23(2) (2009) 811-819)

#### SEP 0913

"Phase Equilibria Modeling of Methanol-Containing Systems with the CPA and PC-SAFT Equations of State" Peter Chr. V. Tybjerg, Georgios M. Konto-

## georgis, Michael L. Michelsen, and Erling H. Stenby

(Fluid Phase Equilibria, 288(1-2) (2010) 128-138)

#### SEP 0914

"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 0915

"Errata: "Evaluation of the Nonrandom Hydrogen Bonding (NRHB) Theory and the Simplified Perfurbed-Chain-Statistical Associationg Fluid Theory (sPC-SAFT). 2. Liquid-Liquid Equilibria and Prediction of Monomer Fraction in Hvdrogen Bonding Systems" Ioannis Tsivintzelis, Andreas Grenner, Ioannis G. Economou, and Georgios M. Kontogeorgis (Industrial and Engineering Chemistry Research, 48(16) (2009) 7860)

#### SEP 0916

"Modelling of Phase Equilibria with CPA using the Homomorph Approach" Martin P. Breil, Ioannis Tsivintzelis, and Georgios M. Kontogeorgis (Accepted by Fluid Phase Equilibria)

#### SEP 0917

"Extended UNIQUAC Model for Thermodynamic Modeling of CO<sub>2</sub> Absorption in Aqueous Alkanolamine Solutions" Leila Faramari, Georgios Kontogeorgis, Kaj

Thomsen, and Erling H. Stenby (Fluid Phase Equilibria, 282 (2009) 121-132)

#### SEP 0918

"Estimation of the Impact of Sulfur Species on Glycol Dehydration" Waheed Afzal, Martin P. Breil, Amir H. Mohammadi, Georgios M. Kontogeorgis, and **Dominique Richon** 

(Presented at EQUIFASE 2009, Porto, Portugal)

#### SEP 0919

"Experimental Study and Phase Equilibrium Modeling of Systems Containing Acid Gases and Glycols using the Cubic-Plus-Association EoS"

Waheed Afzal, Martin P. Breil, Ioannis Tsivintzelis, Amir H. Mohammadi, Georgios M. Kontogeorgis, and Dominique Richon (Submitted to Fluid Phase Equilibria)

#### SEP 0920

"Modeling Phase Equilibria for Acid Gas Mixtures using the CPA Equation of State. Part I. Mixtures with H2S" Ioannis Tsivintzelis, Georgios M. Kontogeorgis, Michael L. Michelsen, and Erling H.

Stenby (Accepted by AIChE Journal)

SEP 0921 "Absorber Model for CO<sub>2</sub> Capture by Monoethanolamine"

Leila Faramarzi, Georgios M. Kontogeorgis, Michael L. Michelsen, Kaj Thomsen, and Erling H. Stenby

(In press in Industrial and Engineering Chemistry Research)

#### SEP 0922

"Teaching Chemical Engineering Thermodynamics at Three Levels" Georgios M. Kontogeorgis, Michael L. Michelsen, and Karsten H. Clement (Chemical Engineering Education, (2009) 70-78)

#### SEP 0923

"The Effects of Possible Contamination on the Radiocarbon Dating of the Dead Sea Scrolls II: Empirical Methods to Remove Castor Oil and Suggestions for Redating"

Kaare Lund Rasmussen, Johannes van der Plicht, Gregory Doudna, Frederik Nielsen, Peter Højrup, Erling Halfdan Stenby, and Carl Th Pedersen

(Radiocarbon, 51(3) (2009) 1005-1022)

SEP 0924 "CO<sub>2</sub> Capture from Flue Gas using Amino Acid Salt Solutions" Benedicte Mai Lerche, Erling H. Stenby, and

Kaj Thomsen (Proceedings from Risø International Energy Conference 2009)

#### SEP 0925

Alkanolamine Systems"

SEP 0926 Coefficient Models" Stenby

SEP 0927 Stenby 252, Roskilde, Denmark)

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

#### SEP 0929

Thermodynamic Modeling of Water-Acid Gases-

Negar Sadegh, Kaj Thomsen, Erling H. Stenby, and Georgios Kontogeorgis (Oral presentation at 9th AIChE Annual Meeting, Nashville, TN, November 2009)

"Thermodynamics of Irreversible Processes Enhanced by Mixed Solvent Electrolyte Activity

Philip L. Fosbøl, Kaj Thomsen, and Erling H.

(Poster presentation and proceedings from JETC10, (2009) Copenhagen, Denmark)

"Energy Demand for CO<sub>2</sub> Solvent Regeneration" Philip L. Fosbøl, Kaj Thomsen, and Erling H.

(Oral presentation and proceedings from Risø International Energy Conference, (2009) 242-

136)

"1D Simulations for Microbial Enhanced Oil Recovery with Metabolite Partitioning" Sidsel M. Nielsen, Alexander A. Shapiro, Michael L. Michelsen, and Erling H. Stenby (Submitted to Transport in Porous Media)

## CERE Staff 2009-2010

Faculty	Ida Lykke Fabricius Georgios Kontogeorgis Michael L. Michelsen Klaus Mosegaard Alexander A. Shapiro Nicolas von Solms Erling H. Stenby, Director Kaj Thomsen
Scientific Staff	Martin P. Breil, Assistant Professor Birgit Elkjær Ascanius, Research Assistant Philip L. Fosbøl, Assistant Professor Jan Frydendall, Post Doc Thomas Mejer Hansen, Post Doc Peter Jørgensen Herslund Matias Alfonso Monsalvo, Post Doc Saravanan Swaminathan, Post Doc Ioannis Tsivintzelis, Post Doc Duc Thuong Vu, Engineer Wei Yan, Associate Professor Yi Lin, Post Doc Vasu Neela, Research Assistant Subham Paul, Post Doc André Fettouhi, Post Doc
Technical and Administrative Staff	Povl Valdemar Andersen, Laboratory Technician Anne Louise Biede, Secretary Mia Trolle Borup, Center Coordinator Christian Carlsson, IT-Coordinator Thoung Dang, Laboratory Technician Karin Petersen, Laboratory Manager Zacarias Tecle, Laboratory Technician Patricia Wagner, Secretary
PhD Students	Mohammad Monzurul Alam Ahmed Awadelkarim Ane Søgaard Avlund Rasmus Risum Boesen Knud Cordua Victor Darde Leila Faramarzi José Fonseca Zakir Hossain Priyanka Jain Lars Jensen Katrine Lange Benedicte Mai Lerche Rasmus Lundsgaard Sidsel Marie Nielsen Ben Niu Muhammad Riaz Negar Sadegh Sara Sandersen Carsten Völker Hao Yuan Adeel Zahid Xuan Zhang
External PhD Students	Ulrik Ankergren Rudi Pankratz Nielsen Janne Fritt-Rasmussen
Guests	Waheed Afzal, Visiting PhD Student Javeed Awan, Visiting PhD Student Elsa Moggia, Visiting Post Doc Alfonso Tapia, Erasmus Student Riian de Villiers, Visiting MSc. Student Carole Langlais, Erasmus Student
Laboratory Tranies	Emine Yüksel Randi Neerup
Other Staff	Trevor Jagerfield, Student Worker Bjørn Maribo-Mogensen, Student Worker Hao Yuan, Student Worker