DTU

Annual Report 2008

IVC-SEP

Center for Phase Equilibria and Separation Processes

Department of Chemical
and Biochemical Engineering

Technical University of Denmark

Contents

Photo: StatoilHydro

Entering New Strategic Fields

IVC-SEP celebrates its 30 years of existence in a research funding climate where independent research is not given high priority. Fortunately we are able to engage in new fields without jeopardizing long term continuity

Applied thermodynamics is an important ingredient in most innovative products and processes. Celebrating the 30 year anniversary of IVC-SEP, we can look back at a wide range of applications. While this variety has largely been research interest driven, today we can be grateful to the flexibility it provides us, as we realize that the funding situation in Denmark will influence the future direction of IVC-SEP projects.

Default budgets of Danish universities are not growing and independent research funding is not given high priority. Instead an increasing part of public research funding is directed towards strategic themes with high political attention. Fortunately a number of these strategic themes are within our natural sphere of interest, meaning we have been able to step into new areas without jeopardizing long term continuity.

A new generation of CPA Equations of State and sPC-SAFT to complex applications where traditional tools cannot be utilized is one example of the constant development of new models. Similarly the Extended UNIQUAC model – becoming applicable to more and more electrolyte systems - is an example of existing models being extended.

As shown in the present report, the IVC-SEP industry Consortium continues to evolve, attracting new members and engaging long standing members further in projects of mutual interest. The continued evolvement of the Consortium is a proof of the strength and vitality of the centre even after three decades.

We are convinced that it is the combination of continuity and the ability to step into new areas that makes us an attractive collaborator for academic and industrial partners. Thus we will continue to focus on the quality of ideas and the relevance of our work to the development of the engineering sciences.

Professor Erling Stenby,
Director of IVC-SEP

Erling Stenby
Director of IVC-SEP,
professor
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A more detailed summary of 2008 events to be found at page 14.

IVC-SEP Konsortium:

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

The Consortium - our Strongest Asset

The IVC-SEP 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 Centre is supported by grants from several private companies. The strongest asset of the IVC-SEP 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 Centre. This ensures that IVC-SEP 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 IVC-SEP research at the highest international level.

With the courtesy of ConocoPhillips

ConocoPhillips finds, produces, refines, markets and ultimately supplies energy resources to individuals and businesses worldwide.

We welcome...

ConocoPhilips: As the third-largest integrated energy company in the United States, based on market capitalization, oil and natural gas reserves, ConocoPhillips finds, produces, refines, markets and ultimately supplies energy resources to individuals and businesses worldwide. As of December 2008, the company's refineries included 12 in the United States, four in Europe and one in Asia. The worldwide refining capacity was 2.67 million BPD (barrels per day).

ConocoPhillips' assets include natural gas operations and related business conducted through its 50 percent interest in DCP Midstream. As of December 2008, the company had 63 natural gas processing plants and approximately 60,000 miles of gathering lines.

ConocoPhillips also participates in chemicals and plastics production worldwide through its 50 percent interest in Chevron Philips Chemical Company (CP Chem), one of the world's largest producers of olefins, polyolefins, aromatics and styrenics, piping and proprietary plastics. As of December 2008, CP Chem had five research centers and 35 production facilities in nine countries.

Gassco: Owned wholly by the Norwegian state, Gassco is the operator for the integrated system for transporting gas from the Norwegian continental shelf to other European countries. The company was established May 2001 and soon after took over the operatorship for all gas transport from the Norwegian shelf.

During 2008 Gassco delivered a total volume of 94.6 billion kubic meters of gas to receiving terminals plus a total volume of 8.6 million tonnes of other products – primarily ethane, propane, butanes, naphtha and condensate (light oil). Gassco does not make a profit or a loss from its own operations. The cost of operating the transport system is met by its users through tariff payments.

INEOS: In a relatively short time span, INEOS has grown to become the world's third largest chemical company. The company is a global manufacturer of petrochemicals, specialty chemicals and oil products. Employing a total of 15,500 it comprises 17 businesses each with a separate chemical company heritage. INEOS' production network spans 64 manufacturing facilities in 14 countries throughout the world. The total production volume is 57 million tonnes.

The rapid growth is partly due to acquisitions. INEOS' pedigree includes Amoco, BASF, Bayer, Borealis, BP, Degussa, Dow, Enichem, Erdölchemie, Hoechst, ICI, Innovene, LANXESS, Monsanto, Norsk Hydro, Solvay and Union Carbide.

Lloyd's Register ODS: Based on a strong foundation in research and development, Lloyd's Register ODS specializes in advanced engineering simulation technology for the design and analysis of complex structures and systems – across business streams such as marine, oil & gas, utilities & power, transportation, engineering & construction and defence. The company has delivered practical solutions to difficult engineering problems for over 50 years. With offices in Denmark, Sweden, Norway, England, France, China and Canada, Lloyd's Register ODS employs more than 150 consultants worldwide.

Advanced Recovery - Huge Potential, Huge risk

As the world's oil fields have an expected average recovery rate of less than 50 per cent, the potential economic and energy supply benefits of successful Enhanced Oil Recovery (EOR) are eminent. In-Situ Combustion and use of surfactants – either factory produced or from microbes at the site – are novel, advanced EOR techniques.

Enhanced Oil Recovery (EOR) is a way to extend the productive life of an otherwise depleted and uneconomic oil field. Most commonly either a gas or a liquid substance is injected into the reservoir – however the range of potential EOR techniques also includes thermal methods like In-Situ Combustion and microbiological methods. EOR is usually applied after more conventional methods, primarily pressure depletion and water flooding, have been exhausted.

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IVC-SEP's project ADORE (Advanced Oil Recovery Methods) focuses on some of the most advanced EOR methods. The use of surfactants – chemical flooding – and In Situ Combustion hold huge potentials for enhancing oil recovery but also represent high costs and high risk.

The project is even more relevant to the Danish oil fields where the recovery rate due to the geological conditions is expected to be below 30 per cent. This has attracted sponsorships from the Danish Research Council for Technology and Production Sciences and from Maersk Oil and from DONG Energy.

"As such a large proportion of the oil resources in the Danish part of the North Sea are expected to be left behind, one also has a large target for EOR. Increasing the recovery rate would be highly desirable. The key question is whether it can be done in an economically feasible way," says Michael Engell-Jensen, Senior Vice President of Maersk Otil.

Besides the sponsorships, Maersk Oil and DONG

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Michael Engell-Jensen, Senior Vice President, Maersk Oil

Energy participates through data supply – just as other members of the IVC-SEP Consortium are expected to.

EOR generally introduces a range of new challenges into oil recovery. For example EOR may cause subsidence in the geological structures. This may actually be an advantage in some cases. You may use subsidence as a tool for making the oil leave its cover – much like squeezing a sponge will give you more soap. On the other hand heavy subsidence could cause the structure to collapse in a way that would block the flow of oil. In other words: subsidence may be positive, but only if it takes place in a controlled manner.

The processes involved in both use of surfactants and In-Situ Combustion are so complex that they cannot be modelled or simulated in a satisfactory manner with present industrial tools. The ADORE project aims at providing a range of novel tools. Efforts are devoted to five core areas: Reactive Transport. Phase Behavior. Porous Media. Rock Mechanics. Numerical Methods.

Each field has a least one PhD project (in total, the ADORE project has eight PhD projects), while two Post Doc's work across fields. Besides IVC-SEP itself two other DTU departments are involved: Informatics and Mathematical Modelling (IMM) and Mechanical Engineering (MEK). Furthermore geotechnical institute GEO participates, just as Stanford University and University of Southern California.

Microbiology EOR: Frontrunner science

While surfactants and In-Situ Combustion are both at the very core of the ADORE project, IVC-SEP Director Erling Stenby mentions microbiological EOR methods as a potential field of increased interest:

"Manipulating microbiology is actually not unknown to the oil industry. For example in some fields, where growth of naturally occurring sulphur-reducing microbes would cause problems, it is an established method to inject nitrate-rich sea water. This stimulates growth of nitrate-reducing microbes which again limits the potential growth of sulphur-reducing microbes. We imagine that similar methods could be used to stimulate growth of microbes that produce surfactants with the ability to decrease oil surface tension which in turn would increase recovery. Actually you might look at this chemical flooding – but with the eminent advantage that the chemical "factory" would be microbes at the site so costs of production, transport and injection of chemicals would be drastically reduced."

DONG Energy sponsors an IVC-SEP project within microbial enhanced oil recovery (MEOR).

"We are working at being able to model these processes. This is yet at a very early state of science – you might call it real frontrunner science," Erling Stenby ads.

Photo: Maersk Oil

Maersk Oil

Maersk Oil and its subsidiary companies are part of the A.P. Møller – Maersk Group.

Maersk Oil is a midsize international oil and gas company operating an oil production of some 650,000 barrels per day and a sales gas production of up to some 1,000 million cubic feet per day. The company has a net equity production exceeding 550,000 barrels of oil equivalents per day from fields in the Danish and British part of the North Sea, offshore Qatar, in Algeria and Kazakhstan.

A Necessary Part of Climate Protection

Ever more often is Carbon Capture and Storage (CCS) mentioned during the negotiations under the United Nations Framework Convention on Climate Change. As an additional bonus the captured CO_2 may be utilized for enhancing oil recovery

In February 2009, on her very first journey as US Secretary of State, Hillary Clinton visited Beijing – and mutual US-China cooperation within Carbon Capture and Storage (CCS) was one of the topics on the agenda. As the international negotiations on climate protection are speeding up, techniques that aim at capturing CO_2 to store it underground are gaining ever more attention. Few imagine a world without use of coal to be realistic, at least not for the next decades. CCS may be a way to meet energy demands without endangering climate.

As an additional bonus CO_2 is among the substances that are relevant for Enhanced Oil Recovery (EOR). When carbon dioxide is pumped into an oil field with adequate pressure it will mix with oil, making it easier to extract. Also the extra pressure added to the field by the pumped carbon dioxide will help in squeezing the reservoir, driving oil from its cover.

Several IVC-SEP industrial consortium members are active in CCS research and development.

Pilot plant in Esbjerg

Three 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. IVC-SEP takes part in the academic support base of the project.

In the facility the CO_2 content of the flue gas is exposed to an amine solution (amines are organic compounds derived from ammonia, NH_3). The mixture is then boiled resulting in the release of CO_2. Finally the CO_2 is compressed to make it ready for storage.

"The Esbjerg pilot project has shown that CO_2 capture is possible. The top priority now is to do this with a smaller consumption of energy in the capture process", says Willy van Well, coordinator of CO_2 capture technology development at DONG Energy.

Vattenfall takes part in the EU technology platform "Zero emission fossil fuel power plants". The vision of the platform is to have one or more CCS technologies commercially available by 2020. An intermediate goal is to have between 10 and 12 demonstration plants operating in Europe by 2015.

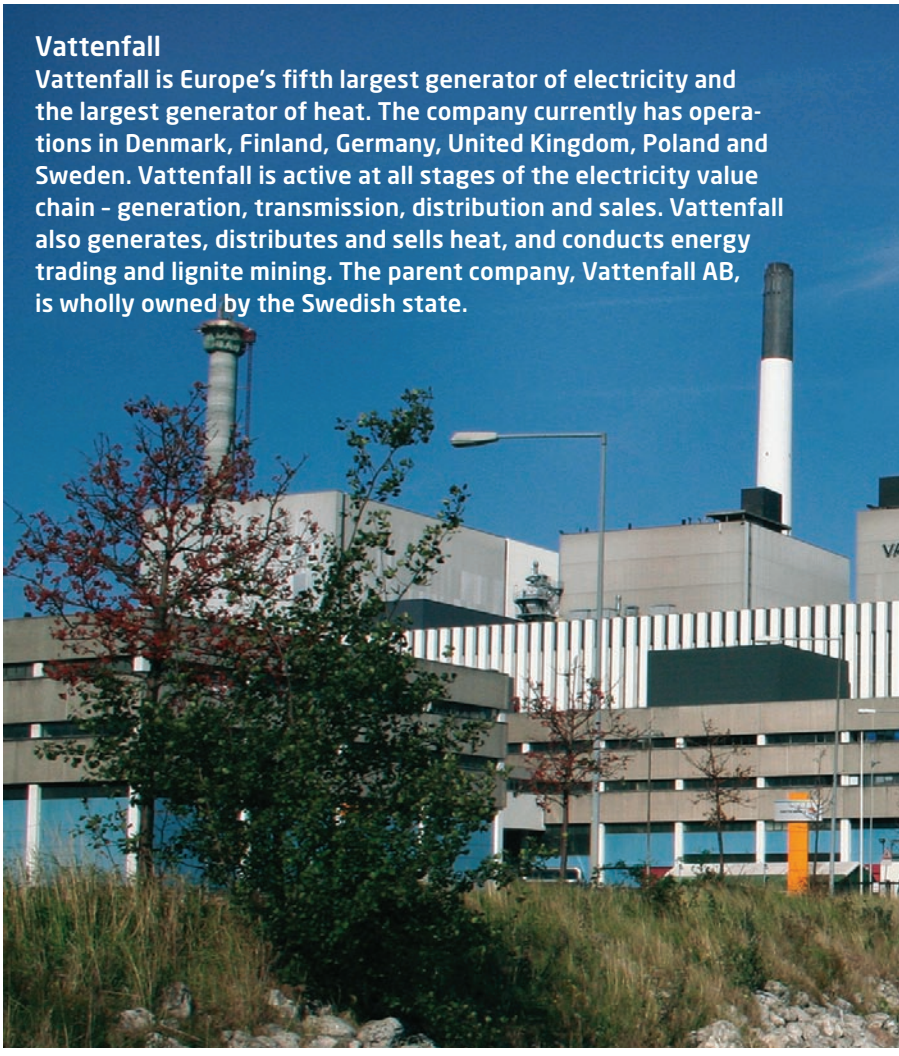
"We are not seeing CCS as replacing neither renewable energy nor energy savings", Hakon Mosbech, Nordic head of engineering at Vattenfall's division Thermal Power, wishes to underline.

"Vattenfall will continue to invest heavily in renewable energy and energy efficient technology. However we

> 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. Another way of putting it is to say that our climate doesn't have time to wait for renewable energy and energy savings to do the job. This leads to the conclusion that CCS will more or less be necessary.
>
> **Hakon Mosbech, Nordic head of engineering at Vattenfall's division Thermal Power.**

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 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.



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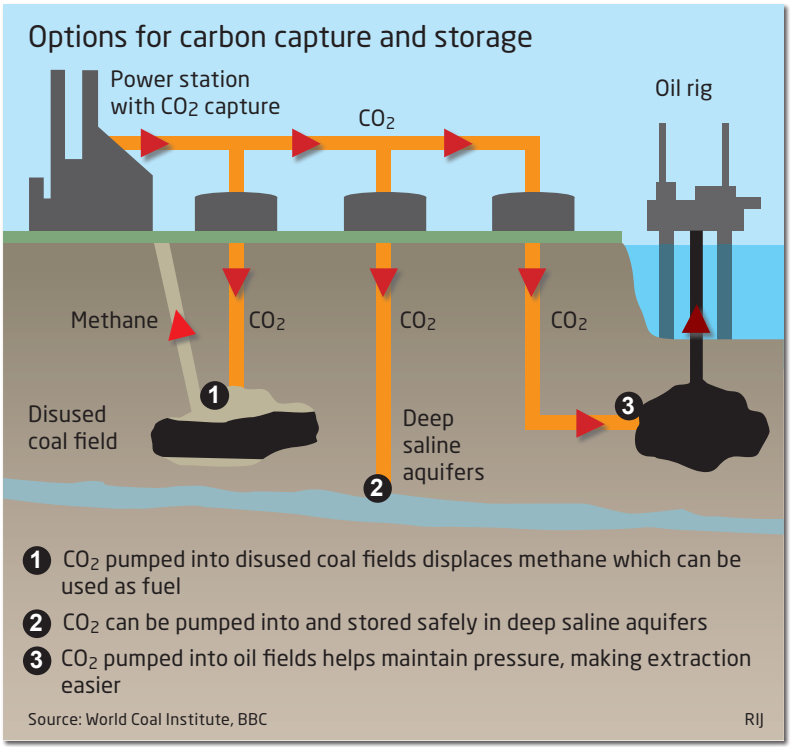
At the Schwarze Pumpe coal fired power plant in Germany Vattenfall has built a pilot plant. Yet we can't expect to see full scale CCS in the near future, Hakan Mosbech feel:

"Besides technological development this would take huge investments. Besi des the expenses of the equipment itself one will have to accept a loss of energy related to capture and storage processes. But renewable energy is expensive as well. In my view CCS should be compared to other types of non-carbon emitting electricity.

Pilot plant at DTU: At DTU Chemical Engineering's test facilities, a 13 meter high pilot plant has been built, in a project where IVC-SEP is involved. The plant simulates carbon capture processes at a fossil fuel power plant.

Photo: Vattenfall



Carbon Capture at IVC-SEP

DONG Energy and Vattenfall jointly sponsor a project on Post-Combustion Capture of CO_2 from Fossil Fuel Power Plants. The aim is to develop design tools for CO_2 absorption / stripping units using aqueous alkanolamines as absorbents. The joint sponsorship covers half of the funding, while the Danish Strategic Research Council covers the other half.

DONG Energy sponsors and leads a project on Enhanced Oil Recovery through CO_2 Utilisation. The purpose is to enhance oil recovery in the North Sea through utilisation of CO_2 captured from a power plant. The project involves multidisciplinary studies including fluid-rock interactions, fluid phase equilibrium and multiphase flow in porous media. The project involves geological research institutions GEO and GEUS plus DTU Environment and Resources. IVC-SEP focuses on phase equilibrium measurements in mixtures of brine, oil and CO_2, modelling and simulating the compositional effects during CO_2 injection into a water flooded oil reservoir, and studies of CO_2 flooding by use of X-ray CT-scanning.

After a smaller study of on The Chilled Ammonia Process for CO_2 Capture an industrial PhD project was started in collaboration with DONG Energy. The Chilled Ammonia Process (CAP) is a relatively new carbon capture process. Initial research has suggested that CAP could be attractive both from an energy perspective and a cost perspective.

GDF-SUEZ, Germany, sponsored two field related studies on utilisation of CO_2 for Enhanced Oil Recovery – in two reservoirs, Knesebeck and Scheerhorn, respectively. The experimental work covers compositional analysis of gas and oil samples, recombination of gas and oil samples to a provided bubbling pressure, constant mass expansion, CO_2 swelling study, check of solid precipitation and reservoir conditions viscosity measurements.

DONG Energy

DONG Energ y is an integrated energy company with leading market positions in Denmark and other key areas of Northern Europe. DONG Energy is a holding company and is incorporated in Denmark. Over the past few years, DONG Energy has shifted its focus from natural gas sourcing, wholesale, exploration and gas and oil production to becoming an integrated energy company with activities across the value chain. Exploration & Production activities are focused in the waters around Denmark, Norway, UK (West of Shetland) the Faroe Islands and Greenland.

In the Witches' Cauldron of Modern Recovery

Current oil recovery depends on a range of chemicals needed to facilitate production, e.g. polymers, surface active substances, emulsion breakers and hydrate inhibitors. These complex mixtures continue to drive development of new chemical theory

The use of a range of oil recovery related chemicals has prompted development of additional chemical theory. Traditionally cubic equations of state (EoS) have been applied to describe phase equalibria in an oil-gas mixture. Cubic equations of state are relatively simple and hold an outstanding track record within gas-liquid phase equilibria solutions related to oil recovery.

Current oil recovery does however depend on a range of chemicals needed to facilitate production, eg. polymers, surface active substances, emulsion breakers and hydrate inhibitors. This calls for adjustment of the cubic equations of state.

Fortunately one does not have to disregard cubic equations of state all together, provided that one includes an additional element which explains the influence of other chemicals involved. IVC-SEP has developed the Cubic Plus Association (CPA) method.

The term refers to cubic equations of state plus an additional element. The additional element is borrowed from SAFT (Statistical Association Fluid Theory), a complex model used to describe hydrogen bonds. While a pure hydrocarbon mixture does not have hydrogen bonds, such bonds prevail in any solution containing water, just as substances like methanol and ethylene glycol – both commonly used as hydrate inhibitors in oil and gas production – contain hydrogen bonds.

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

Meeting demands for environmental reporting

StatoilHydro is one of the companies utilizing the CPA.

"We use the model not only for solving problems related to everyday production like hydrate formation and loss of chemicals but also when looking at potential future projects like water in reservoir gas and hydrate inhibition", dr. Even Solbraa, Discipline Advisor for Gas Quality at StatoilHydro, states.

"Ever more oil and gas production will take place at remote locations, typically offshore and under difficult climate conditions with environmental concerns as a strong focus. In order to meet these challenges StatoilHydro focus on application and further development of knowledge and tools within phase behaviour of both new and well known chemicals."

Practical trials and theoretical work go together in a joint project carried out by StatoilHydro R&D in Trondheim, Norway, and IVC-SEP. Through experiments StatoilHydro refines the models developed by IVC-SEP researchers in the field of phase equilibria related to the complex chemical mixtures involved in contemporary oil recovery.

The CPA method can also be applied for describing the fate of the chemicals. How much has been regained and how much has been lost and emitted to the environment? These data are required in environmental reports and needed to meet demands from environmental authorities.

StatoilHydro
StatoilHydro 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

Complex Mixtures at IVC-SEP

IVC-SEP's involvement in the Cubic Plus Association method is a part of the centre's CHIGP (Chemicals in Gas Processing) project. This Joint Industry Project was initiated in 2004. The CHIGP project aims at the further development and optimization of the CPA model to oil-related mixtures containing gas-hydrate inhibitors like methanol and glycols, high pressure applications as well as phase equilibria for mixtures with other chemicals e.g. acetic acid. Current members are StatoilHydro, GASSCO, Total, BP and Maersk Oil.

StatoilHydro sponsors a project on Distribution of Complex Chemicals in Oil-Water Systems. As crude oil resources decrease, ever more complex chemicals are used in exploitation. Some of these chemicals are added in small quantities, making their detection by chemical analysis difficult. In the project a predictive model for oil-water and octanol-water partition coefficients will be developed and relation between them investigated.

The Danish Research Council for Technology and Production Sciences sponsors a project on Multiphase Equilibrium in Natural Gas / Hydrate Inhibitor Systems. Initially the project will design a new model cell, suitable to be used in a large range of temperatures and pressures, allowing for example the replication of the polar conditions under which some pipelines are used. Further on, the work will include modelling of these systems with equations of state.

Two projects sponsored by DTU are also related to complex mixtures. One project addresses Gas Hydrate Kinetics in Realistic Reservoir Systems and looks at both Formation and Inhibition of gas hydrates. Secondly a project aims for deeper understanding of association models to complex chemicals.

> Efficient and environmentally careful use of chemicals is crucial in oil and gas production.
>
> **Dr. Even Solbraa, Discipline Advisor for Gas Quality at StatoilHydro.**

Photo: Øyvind Hagen, StatoilHydro

experience from the Norwegian continental shelf, pioneering complex offshore projects under the toughest conditions. StatoilHydro has about 29,500 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.

Accumulation and Transport of Mixtures in Micro-porous Solids

The behaviour of fluid mixtures in micro-porous solid materials is becoming increasingly relevant to a number of industrial fields. IVC-SEP has developed a range of new tools, improving both theoretical understanding and practical applications

The behaviour of fluid mixtures in micro-porous solid materials is becoming increasingly relevant to a number of industrial fields. One obvious application is within Enhanced Oil Recovery (EOR) in tight geological structures – e.g. as found in a number of North Sea oil fields. Another application is in catalysts – where one often desires a micro-porous, or even nano-porous structure in order to improve the output per volume unit of catalyst.

However, the range of applications does not stop here. Besides in EOR, fluid mixtures in micro-porous materials are found in other petrochemical fields, in the chemical, food and pharmaceutical industries for pollution control and mixture separation. Porous materials are also important for many practical applications in ecology – e.g. filtering and carbon dioxide sequestration in depleted coal mines; in nanotechnology, storage of natural gas and in hydrology – e.g. flow, adsorption and diffusion of liquids and gases in aquifers.

Confinement of molecules within narrow pores affects both equilibrium and transport properties of the fluid.

The IVC-SEP project Accumulation and Transport of Mixtures in Micro-porous Solids; or MiMics (Mixtures in Micro-porous Solids), has tested the multi component potential theory of adsorption (MPTA) on a large set of gas and liquid mixtures in wide ranges of conditions in micro-pourus solids like activated carbons and zeolites.

The MPTA uses an equation of state (EoS) to describe the equilibrium in multi component fluids;

Enhanced Oil Recovery in tight geological structures is one field where understanding of the behaviour of fluid mixtures in micro-porous solid materials is crucial.

and interaction potential functions to describe the fluid-solid interactions. This makes it possible to generate different MPTA-models by combination of relevant EoS / potentials.

The project has developed and tested a wide range of MPTA-related tools. An experimental database containing more than 2,500 experimental points has been created. The database contains adsorption equilibrium data for single/binary/ternary/quaternary gas mixtures on various porous solids. The database also contains adsorption data for binary/ternary liquid mixtures.

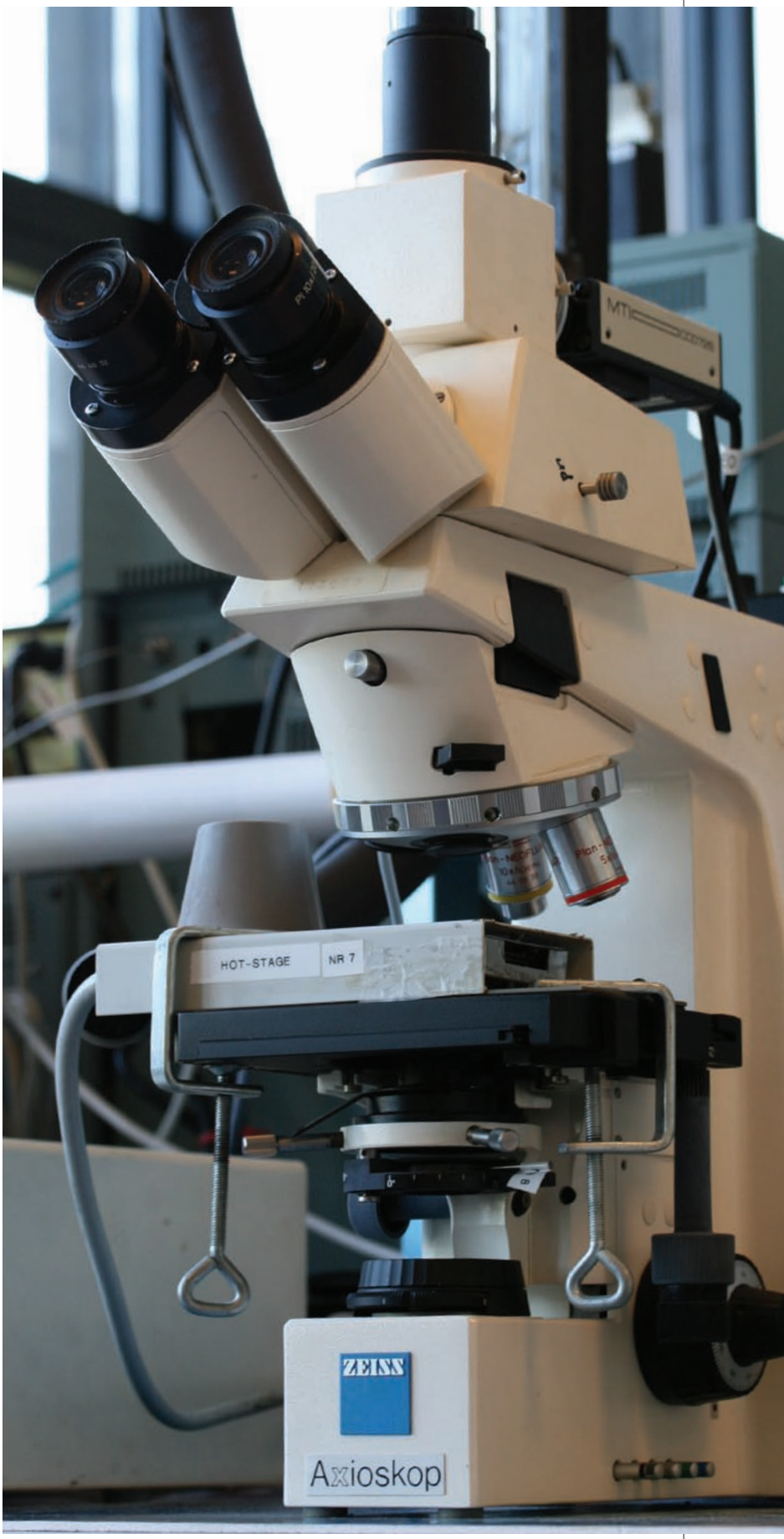
The work has shown that the MPTA can actually predict the behaviour of a large number of mixtures from single-component adsorption data. Also the MPTA is capable of correctly describing complex physical behaviour at high pressures and supercritical conditions. Further, MPTA theory has been extended onto liquid mixtures. The results are satisfactory for engineering applications.

A major part of the project has been dedicated to studies of transport of mixtures in porous solids. Examples of well studied regimes include flows in the continuous regime (viscous flow) and flow of a strongly rarified gas in the so-called Knudsen regime. However, an intermediate regime – very relevant to processes occurring both in porous catalysts and in tight natural gas reservoirs - has not been studied to the same extent. We have derived flow equations for the intermediate regime, including the effects of pressure and thermal gradients.

The studies have included very micro-porous media, where each pore may contain just a few gas molecules. A new random-walk based theory of diffusion in such porous media has been developed. A new described effect – temporal step dispersion – has resulted in a qualitatively correct prediction that more gas molecules than expected will travel further from the injection point; and, simultaneously, more molecules will stay close to this point.

The studies have resulted in an unexpected new development: analysis of the tracer and suspension flows in porous media. This is an important subject in ecological applications (e.g. spreading of contaminants and viruses in the ground), in chemical engineering (filtration and industrial catalysts) and in petroleum engineering (problems of injectivity decline due to well neighbourhood damage). Preliminary work suggests an explanation to experimental observations previously found paradoxical: that the maximum of the concentration moves slower then the carrier convective flux, and that its dispersion is asymmetric and higher than expected.

Software for numerical solutions to the listed problems has been developed.



Highlights from a Busy Year

Erling Stenby
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While presence at the 2008 World Petroleum Congress marked a "first" for IVC-SEP, the year also saw the revival of classic activities such as our thermodynamic models course. Overall the year saw a rise in activity.

In this IVC-SEP Annual Report for 2008 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 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.

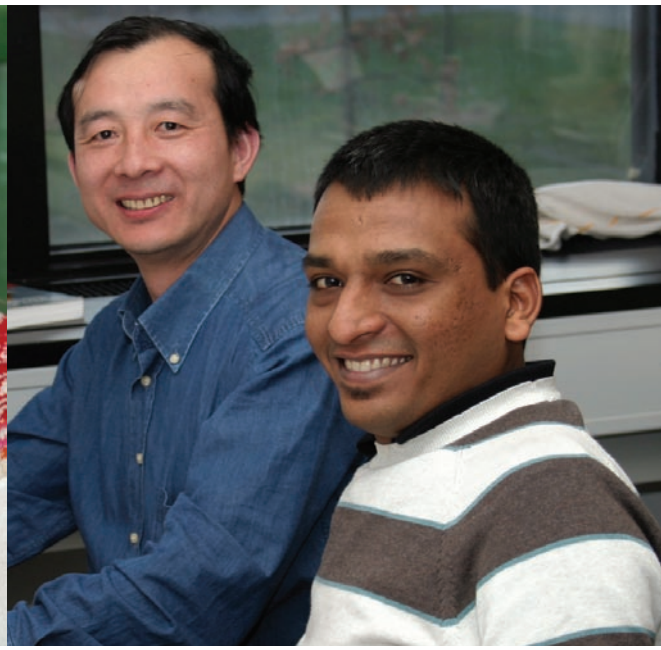
The PhD course "Thermodynamic Models: Fundamentals & Computational Aspects" has been extremely popular every time it has been offered by Michael L. Michelsen and Jørgen Mollerup. In January 2008 it took place again. Our colleagues had set the maximum number of participants at 20, but where overwhelmed by the interest and accepted 27 participants of which almost half came from industry.

In early June we had the pleasure of hosting the PhD course "Molecular Simulation of Complex Chemical Systems with Emphasis to Practical Applications"given by Professor Ioannis Economou from National Center for Scientific Research "Demokritos" in Greece. The course was a part of introducing molecular simulation in our research and education activities. The course had 15 participants and was very successful. Some of our students have already used the new knowledge in their projects.

The annual Discussion Meeting of IVC-SEP took place for the 29th time from 16 to 18 June. The attendance from our member companies was excellent and the interaction between colleagues and external participants as usual very fruitful.

An IVC-SEP first in Madrid

From 30 June to 3 July the World Petroleum Congress took place in Madrid. For the first time IVC-SEP was present with a small booth in the exhibition as part of the Danish national representation. This gave an excellent opportunity to present petroleum research and education activities at the Technical University of Denmark.



The IVC-SEP Consortium continues its positive development. During 2008 we have welcomed the following companies: Lloyd's Register ODS, ConocoPhillips, Ineos, and Gassco. We are very proud that we can attract so many important companies from the chemical and energy industrial sectors. We see this as a confirmation that the research that we undertake is still of high quality and relevance.

We do not collaborate exclusively with the Consortium members. It is important to constantly explore new areas of research. Where do we find the problems that stimulate our curiosity and challenge our scientific instinct? Therefore we are in open dialogue with many non-member companies who maybe need our know-how and research. We discuss collaboration and topics of mutual interest.

Recruitment running smoothly

The pressure on academia to work ever closer with industry is increasing and the discussions about commercial rights, confidentiality, exclusivity, time tables, and deliverables are now a natural part of any scientific collaboration both with companies and other academic institutions. Since IVC-SEP has had excellent relations to industry and have developed a modus operandi of mutual respect and trust we almost always manage to reach an agreement.

One year ago the problem was shortage of scientific staff. Today the situation has changed and we find highly qualified candidates for PhD and Post Doc positions without any problems.

The development has not solved the challenge of handling many small projects. On the contrary we receive an increasing number of requests for short term projects focusing on very specific problems. This requires much attention from the Faculty members and it increases the administrative over head. We also have to initiate larger projects and JIPs such as CHIGP in order to use our resources efficiently.

Major ongoing projects

Below I have listed the major ongoing projects including the level of man power working at IVC-SEP directly on each project:

• LUWS – Liquefaction in Unseparated Well Streams 2008-2010. Collaboration with Institute for Energy Technology in Norway and Statoil. Funded by the

The images display moments captured during Oilsim Course, IVC-SEP Summer School, DM Poster Session, PhD course and other significant 2008 events.

...Highlights from a Busy Year

Norwegian Research Council. 1 Post Doc

• Simulating Reactive Transport in Enhanced Oil Recovery 2006-2010. DTU PhD Scholarship. 1 PhD student (now a part of the ADORE project)

• Environmentally friendly plasticizer 2007-2010. Co-funded project between DTU and Danisco. 1 PhD student

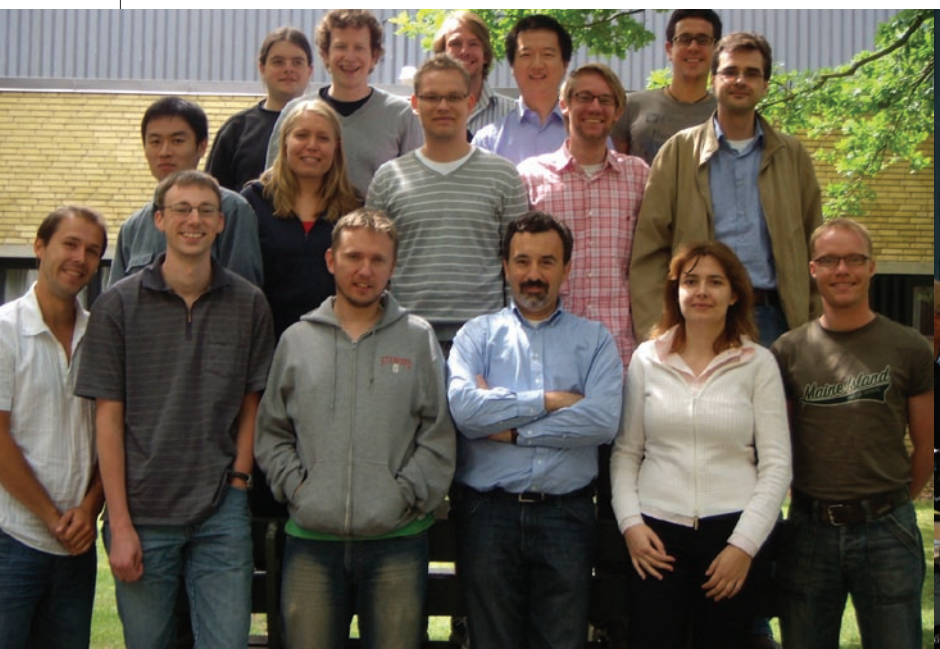
• Gas Hydrates research with focus on inhibitors 2006-2010. Funded by the Danish Research Council for Technology and Production Sciences + DTU. 2 PhD students + 1 Post Doc

• Petroleum refining. 2007-2010. Co-funded project between DTU and Haldor Topsoe. 1 PhD student

• CHIGP II 2007-2012 (originally an acronym for "Chemicals in Gas Processing". Over the years many other applications have been added, but we keep the name). This highly successful JIP which has been running for the last 3 years continued from 1 January 2007. We have commitment from all of the previous participants which were: Statoilhydro, BP, Total, and Maersk Oil. Further more Gassco has joined this project for a 3 year period. 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 PhD scholarship from DTU. 3 PhD students + 2 Post Docs

• ADORE (Advanced Oil Recovery Methods) 2007-2012. A 5 year research project focusing on EOR methods other than gas injection processes. It is supported by The Danish Research Council for Technology and Productions Sciences with EUR 2 mio. This project will have 8 PhD students and 2 Post Docs involved. Maersk Oil and DONG Energy have joined the project as the first industrial sponsors and other member companies have been invited to join as well. The project is a collaboration with two DTU departments (DTU Mechanical Engineering and DTU Informatics) and the independent technology company GEO, specializing in geotechnical problems.

• The last major theme to mention is "CO_2 Captu-



re 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 present tough challenges when it comes to simulation of the actual capture process. In addition to the modelling and simulation work we are involved in the establishment of a pilot plant that is presented in this report. We now have 5 coworkers in this area and we will expand our CCS activities during 2009. Again we welcome collaboration and input from the member companies.

Activity set to remain high

With these projects we have secured a very high level of activity in IVC-SEP for the coming year. My expectation is that it will remain at this level for several years and possibly increase further considering the ongoing negotiations and pending applications submitted to various funding agencies.

At the end of this report you will find an overview of the manuscripts produced by the IVC-SEP coworkers during 2008. Members of the IVC-SEP Consortium can down load all of these from our web site, but anyone can contact us for copies of any of the published papers. Our web site www.ivc-sep.kt.dtu.dk also contains information about our research software, SPECS, our CAPE-OPEN tools and our extensive electrolyte database.

In August 2009 we will once again organize the Summer school "Petroleum Reservoir Fluids Thermodynamics".

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

Research Funding in IVC-SEP

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

The research carried out in IVC-SEP is funded by grants from a number of public and private sponsors. During 2008 our external research funding has increased to a total budget of EUR 2.7 million.

The behaviour of fluid mixtures in micro-porous solid materials is becoming increasingly relevant to a number of industrial fields. One obvious application is within Enhanced Oil Recovery (EOR) in tight geological structures – e.g. as found in a number of North Sea oil fields. Another application is in catalysts – where one often desires a micro-porous, or even nano-porous structure in order to improve the output per volume unit of catalyst.

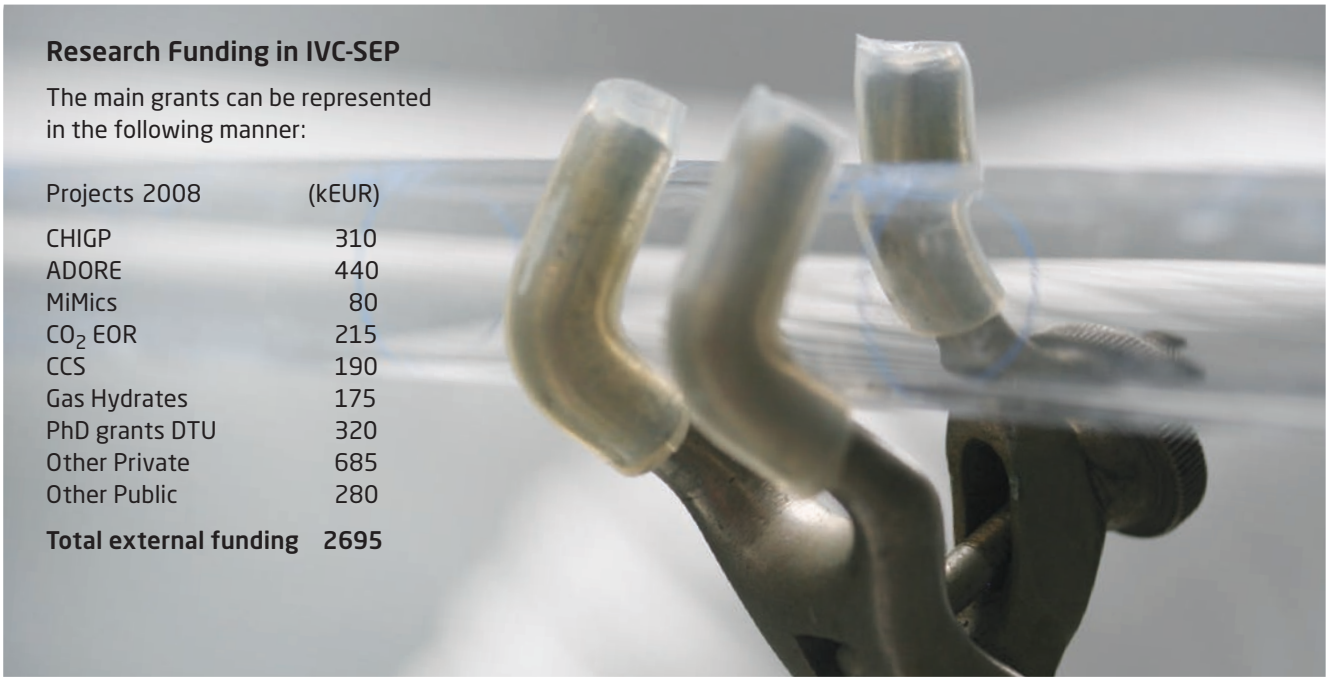
However, the range of applications does not stop here. Besides in EOR, fluid mixtures in micro-porous

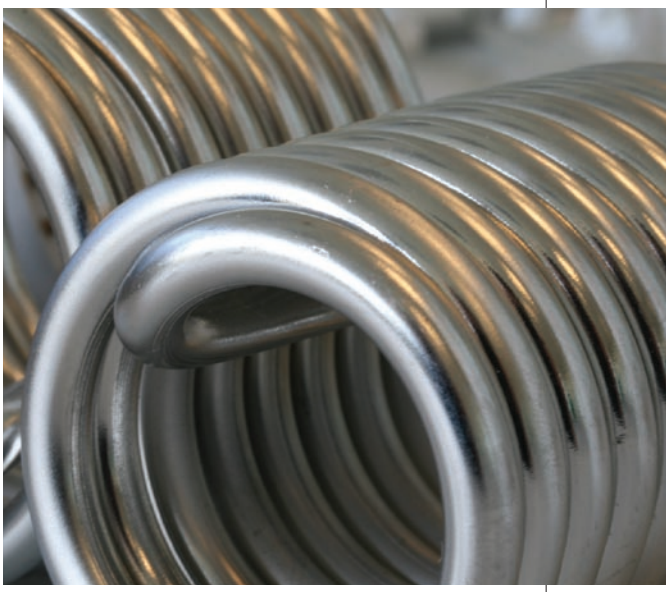
The item Other Private covers a wide range of projects and we are happy to enter into close and challenging collaboration with our member companies. On the other hand we have also learned that the administrative effort and the paper work needed to establish a small formal collaboration is close to the same as that needed for a large formal collaboration. We therefore try to limit the number of small projects in order to minimize the bureaucratic overhead and to secure that the limited resource consisting of the supervising capacity of the Faculty is spent in the most meaningful manner possible. When it comes to the legal agreements I would like to acknowledge the highly qualified support we receive from the DTU central legal office.

Research Funding in IVC-SEP

The main grants can be represented in the following manner:

Projects 2008	(kEUR)
CHIGP	310
ADORE	440
MiMics	80
CO_2 EOR	215
CCS	190
Gas Hydrates	175
PhD grants DTU	320
Other Private	685
Other Public	280
Total external funding	**2695**





Carbon Dioxide Corrosion: Modelling and Experimental Work Applied to Natural Gas Pipelines

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The main objective of the thesis is to improve understanding of the CO_2 corrosion mechanism with special emphasis on wet gas pipelines for transportation of natural gas offshore. CO_2 corrosion is a general problem in industry leading to considerable costs.

While a number of models for prediction of CO_2 corrosion are available in the literature, these models are not very accurate and assume ideality in the main part of the equation. This is a crude assumption as the ionic strength is up to 10 in certain pipelines.

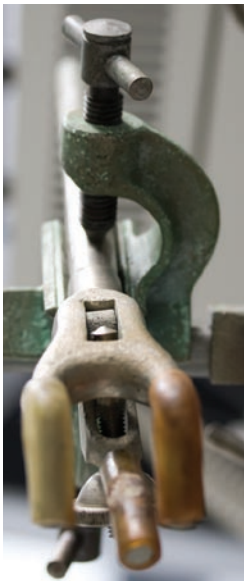
This thesis aims to improve the models and take non-ideality into account. A thermodynamic model is built. Parameters for the extended UNIQUAC model are presented for the extension to MEG calculations in the multi solvent electrolyte system: CO_2-$NaHCO_3$-Na_2CO_3-MEG-water. Parameters are regressed to literature values of SLE, VLE, heat excess and validated for heat capacity data.

212 experimental SLE data points were measured and used in the thermodynamic modelling. The determined parameters are valid between -50 and 90 degrees C.

A model of the density in the CO_2-$NaHCO_3$-Na_2CO_3-MEG-water system is given from literature values and experimental work measured in this study. The model is valid between 2 and 60 degrees C.

A database of approximately 3,500 data points on phase equilibrium measurements in systems containing CO_2, CH_4, MEG, DEG, TEG and water was collected and evaluated. The thermodynamic factors have been calculated in the system CO_2-$NaHCO_3$-Na_2CO_3-MEG-water. The results show that diffusivities of Na^+, HCO_3^-, CO_3^{2-}, MEG and CO_2 (aq) may vary 60 % up or down compared to the infinite dilute diffusivities. The outcome is independent of whether NaOH, $NaHCO_3$ or Na_2CO_3 is used. The effect on Na^+ diffusivity is high in all cases and MEG is affected at low MEG concentrations. The system seems to perform more ideally in terms of diffusion at high MEG concentrations. CO_3^{2-} diffusivity is a strong function of temperature and partial pressure of CO_2. Diffusivity of CO_2 (aq) is also affected at high CO_2 pressure.

The work shows that all mechanistic CO_2 corrosion models may be improved by applying a thermodynamic model.



Development of Models and Algorithms for the Study of Reactive Porous Media Processes

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PhD
Today works with Schlumberger, Great Britain

In-Situ Combustion (ISC) is a process for enhanced oil recovery (EOR) which is especially relevant as a recovery method for the world's vast heavy oil reserves. Current mathematical models and numerical simulators have shortcomings in providing accurate, efficient and reliable performance predictions required for safe and cost-effective design of ISC projects.

ISC is a complex process coupling chemical reactions and phase equilibria with thermal, multi component multiphase media flow. Accurate prediction of field performance requires that both spatial and temporal resolution in a numerical simulation is adapted. Efficient computational methods are needed.

Two ISC models have been developed. The Virtual Combustion Tube (VCT) is an equation of state compositional, one-dimensional ISC model for laboratory scale combustion simulation. It accounts for the simultaneous flow, transport of heat and mass, chemical reactions and phase equilibrium. The Virtual Kinetic Cell (VKC) models a multi phase chemical batch reactor which facilitates the isolated study of chemical reactions and phase behaviour. Together the two models provide a flexible platform for the fundamental study and support of laboratory scale combustion experiments.

The efficiency of ISC processes depends critically on the formation and sustained propagation of a high-temperature combustion front. The models were employed to study the impact of phase behaviour modelling on ignition / extinction phenomena. Compositional changes affect the chemical kinetics and thereby the process performance. It was demonstrated that a simplified ideal mixture based approach to phase behaviour modelling, which is common in thermal simulators, may overestimate the air injection rate required to sustain combustion compared to a rigorous equation of state based approach.

A simple scheme was proposed for numerical integration of the ISC equations. A family of tailored methods was designed for chemical reaction sub processes. The new methods proved 2-5 times faster than off-the-shelf ODE solvers when applied to operator splitting integration of ISC kinetics. The methods were further extended with a novel algorithm which was shown to improve the integration robustness by lowering the number of convergence and error test failures when crossing phase boundaries.

Statistical Methods for History Matching

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DOND Energy

Fig.1: Reference permeability field. Blue color indicates low permeable mud and red indictes high permeable sand. Production is taking place in vertical wells and injection takes place in a vertical and a horizontal well.

History matching is an important part of oil field management. The term refers to adjusting a reservoir model so that simulated and actual measured production matches. The reservoir model is adjusted until the production history is identical or close to the production calculated by a numerical fluid flow simulation. The reservoir model is mainly used to forecast future production which is crucial for field management. By adjusting the model to match the field's production history one increases the predictive capability of the model. The thesis both evaluates a number of existing history matching techniques and proposes a novel technique.

The proposed method is a hybrid method based on the probability perturbation method (PPM). The method seeks to improve the convergence of the probability perturbation method by including qualitative gradient information. The qualitative information is extracted from the gradient of the objection function by a simple filter which filters out numerically small elements of the gradient. A new parameter denoted "degree of trust" is introduced. This parameter is used to control the impact of gradient information. If this parameter is set to zero the proposed method reduces to traditional probability perturbation.

The proposed method has been applied to history matching examples in 2D as well as in 3D. In all cases the method performs better than traditional PPM, yielding lower end values of the objective function. The gradient-guided method reaches the final value in less iterations. This may be due to regularization effects as well as the qualitative information extracted from the gradient. An existing framework for traditional PPM can easily be extended to include the gradient guidance. This, however, requires that an efficient calculation of sensitivities of production data with respect to reservoir parameters is available. In the current setup an efficient additional method is applied to calculate these sensitivities.a

Fig. 1.

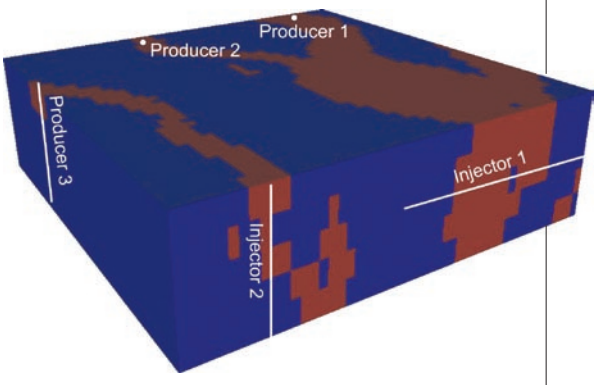

Photo: Colourbox

Development of Soft Nanocarriers from Novel Amphiphilic Hyaluronic Acid Derivatives towards Drug Delivery

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PhD
Today works with
Novozymes A/S

Drug delivery is an important pharmaceutical research area currently facing limitations such as drug insolubility and instability in biological media, poor bio availability and unspecific targeting. As a consequence, high doses are used to achieve a therapeutic effect. This increases the risk for toxicity in patients and increases health costs. The design of advanced drug delivery systems addressing these challenges becomes increasingly important.

This thesis focuses on hyaluronic acid (HA) as a vehicle for drug delivery. HA is a natural linear glycosaminoglycan ubiquitous and identical in all mammals. Due to its native intrinsic biocompatibility, resorbability and biological functions, and the possibility for an easy chemical functionalization, HA constitutes an excellent starting material for the design of advanced biomaterials.

The objective of this project was to develop HA-based nano carriers for encapsulation and delivery of hydrophobic drugs. However, due to its high hydrophilicity, HA exhibits physicochemical properties incompatible with spontaneous and stable formation of segregated structures in aqueous solutions. Therefore, HA was first rendered amphiphilic by covalent binding of hydrophobic groups onto its backbone.

After an investigation of two alternative modification methods, the proprietary technology eventually selected was based on the grafting of octenyl succinic anhydride and was optimised so as to develop a reproducible and robust process for the synthesis of functionalized polymers. A number of fundamental properties were studied. Submicronic multiphasic physically crosslinked nano-gel particles capable of solubilising a model hydrophobic substance were prepared by spontaneous self-association and characterized.

In conclusion, a molecular method based on controlled self-association was developed for formation of HA soft nano structures. These represent novel and promising bio material templates which could be valuable to industry since the underlying production methods are aqueous and easy to scale up

The project was a cooperation between IVC-SEP (DTU), Novozymes Biopolymer A/S and Department of Pharmaceutics and Biopharmaceutics, University of Geneva, Switzerland.

Group Contribution sPC-SAFT Equation of State

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PhD
Today works with
Sika Denmark

Modelling of thermodynamic properties and phase equilibria with equations of state (EoS) is an important issue in chemical and related industries. The simplified Perturbed Chain-Statistical Associating Fluid Theory (sPS-SAFT) EoS is widely used for various industrial applications.

Key parameters of the equations are typically fitted to experimental vapour pressure and liquid density data. Since high-molecular-weight compounds, like polymers, do not have a detectable vapour pressure, there is a need for a predictive calculation method for parameters of polymers and other complex compounds. This thesis suggests a solution to this problem.

The project has developed a group-contribution (GC) version of the sPC-SAFT EoS where parameters are calculated from a predefined GC scheme. In this way, the PC-SAFT parameters for complex compounds can be estimated when experimental data are unavailable.

The PC-SAFT parameter table is extended with over 500 newly estimated parameter sets for pure non-associating compounds from mainly these chemical families: alkanes, branched alkanes, alkenes, alkynes, benzene derivatives, gases, ethers, esters, ketones, cyclo- and fluorinated hydrocarbons, polynuclear aromatics, nitroalkanes, sulphides and plasticizers.

Further testing is needed to establish the real potential of the GC sPC-SAFT EoS. However, the current work has already shown that with the newly developed GC scheme in hand to calculate parameters for complex compounds, the sPC SAFT model has become a relevant and useful engineering tool for the design and development of complex products. These include detergents, food ingredients, pharmaceuticals and speciality chemicals, where predictions of thermodynamic and phase equilibria properties are required, but for which required vapour pressure and/or liquid density data may not be available.

Conference Contributions and Invited Speakers 2008

Ane Søgaard Avlund:
Poster presentation: Application of an Association Model to Alkanolamines, Ane Søgaard Avlund, Georgios M. Kontogeorgis, and Michael L. Michelsen, the 23rd European Symposium on Applied Thermodynamics (ESAT), Cannes, France, 29 May to 1 June, 2008
Oral presentation: Application of an Association Model to Complex Fluids, Ane Søgaard Avlund, Georgios M. Kontogeorgis, and Michael L. Michelsen, 2008 AIChE Annual Meeting, Philadelphia, PA, USA, November, 2008

Rasmus Risum Boesen:
Poster presentation: Competitive Adsorption of Nitrogen Compounds in Hydrodesulfurization of 4,6-dimethyldibenzothiophene, Rasmus Risum Boesen, Kim G. Knudsen, Nicolas von Solms, and Michael Locht Michelsen, 19th World Petroleum Congress, Madrid, Spain, June 29th to July 3rd, 2008

Martin Breil:
Oral presentation: The osmotic second virial coefficient and the Gibbs energy function, Jørgen M. Mollerup, and Martin Breil, the 23rd European Symposium on Applied Thermodynamics (ESAT), Cannes, France, 29 May to 1 June, 2008
Poster presentation: Designing with CAPE-OPEN, Martin Breil, Jostein Gabrielsen, Nicolas von Solms, Georgios M. Kontogeorgis, and Erling H. Stenby, the 23rd European Symposium on Applied Thermodynamics (ESAT), Cannes, France, 29 May to 1 June, 2008
Oral presentation: CAPE-OPEN at IVC-SEP, Martin Breil, CO-LaN Annual General Meeting, Cambridge, UK, 3-4 April, 2008

Victor Darde:
Oral presentation: Chilled ammonia process for CO2 capture, Victor Darde, Kaj Thomsen, Willy J.M. van Well, and Erling H. Stenby, The 9th International Conference on Greenhouse Gas Control Technologies (GHGT9), Washington DC, USA, November, 2008
Oral presentation: Chilled ammonia process for CO2 capture, Victor Darde, Kaj Thomsen, Willy J.M. van Well, and Erling H. Stenby, ICPWS XV conference, Berlin, Germany, September, 2008

Leila Faramarzi:
Oral presentation: The Extended UNIQUAC Model for Prediction of Vapor-liquid Equilibria of Carbon Dioxide in Alkanolamine Solutions, Leila Faramarzi, Georgios M. Kontogeorgis, Kaj Thomsen, Erling H. Stenby, The 9th International Conference on Greenhouse Gas Control Technologies (GHGT9), Washington DC, USA, November 2008
Oral presentation: The Extended UNIQUAC Model for Prediction of Vapor-liquid Equilibria of Carbon Dioxide in Alkanolamine Solutions, Leila Faramarzi, Georgios M. Kontogeorgis, Kaj Thomsen and Erling H. Stenby, 15th International Conference on the Properties of Water and Steam (ICPWS), Berlin, Germany, September 2008

Philip L. Fosbøl:
Poster presentation: Phase equilibria and CO_2 Corrosion - A new approach to corrosion modelling, Philip L Fosbøl, Kaj Thomsen, and Erling H. Stenby, Copenhagen SPE meeting, January, 2008
Poster presentation: Capture and storage project at IVC-SEP, DTU Chemical engineering, Philip L. Fosbøl, DTUEnergy conference, December, 2008

Lars Jensen:
Oral presentation: Propane Gas Hydrate Nucleation Kinetics: Experimental Investigation and Correlation, Lars Jensen, Kaj Thomsen, and Nicolas

von Solms, 6th International Conference on Gas Hydrates, Vancouver, Canada, July, 2008

Rasmus Lundsgaard:
Poster presentation: Estimation of migration and diffusion coefficients of GRINDSTED® SOFT-N-SAFE from PVC into iso-octane, Rasmus Lundsgaard, Georgios M. Kontogeorgis, Jørgen K. Kristiansen and Torkil F. Jensen, 4th International Symposium on Food Packaging, Prague, Czech Republic, 19-21 November, 2008

Matias Monsalvo:
Poster presentation: Behavior of Fluid Mixtures in Porous Materials, Matias A. Monsalvo, and Alexander A. Shapiro, SPE Meeting, Hellerup, Denmark, 25th March, 2008
Poster presentation: Phase Behavior in Confined Systems, Matias A. Monsalvo, and Alexander A. Shapiro, NanoDay 2008, University of Copenhagen, Copenhagen, Denmark, 16th April, 2008

Rudi P. Nielsen:
Oral presentation: Thermodynamic Modeling of Production of Biofuel by Catalytic Conversion at Near Critical Conditions in Aqueous Solution, Rudi P. Nielsen, Steen B. Iversen, Tommy Larsen, Kaj Thomsen, Nicolas von Solms, and Erik G. Søgaard, 16th European Biomass Conference and Exhibition, Valencia, Spain, June, 2008

Nicolas von Solms:
Oral presentation: Refrigeration Plants using Carbon Dioxide as Refrigerant: Measuring and Modelling the Solubility, Diffusivity and Permeability of Carbon Dioxide in Polymers used as Packing and Sealing Materials, Nicolas von Solms, and Vasu Neela, Sixth International Conference on Heat Transfer, Fluid Mechanics and Thermodynamics, Pretoria, South Africa, July, 2008
Oral presentation: Measuring and Modeling the Solubility, Diffusivity and Permeability of Carbon Dioxide in Polymers Used as Packing and Sealing Materials in Carbon Dioxide Refrigeration Plants, Nicolas von Solms, Vasu Neela, and Jakob Kristensen, AIChE Annual Meeting, Philadelphia, PA, USA, November, 2008
Oral presentation: Modelling Hydrogen-Bonding Fluid Mixtures Using Insight Gained from Spectroscopy, Nicolas von Solms, Lars Jensen, Michael L. Michelsen, and Georgios M. Kontogeorgis, AIChE Annual Meeting, Philadelphia, PA, USA, November, 2008
Oral presentation: Which Polymers should be used in Heat Pumps and Refrigeration Systems that use CO_2 as Refrigerant, K. Frederiksen, Nicolas von Solms, Vasu Neela, and Jakob Kristensen, 8th IIR Gustav Lorentzen Conference on Natural Working Fluids, Copenhagen, Denmark, September, 2008

Kaj Thomsen:
Oral presentation: Production of valuable, inorganic salts from fly-ash from biomass combustion, Kaj Thomsen, 16th European Biomass Conference & Exhibition, From Research to Industry and Markets, Feria Valencia – Convention and Exhibition Centre, Valencia, Spain, 2 - 6 June 2008
Invited speaker: Thermodynamic modelling of phase equilibria and thermal properties of the CO_2 – NH_3 – H_2O system, CSIRO PCC Science & Technology Seminar, Aqueous ammonia for post-combustion capture (PCC), Newcastle Energy Centre, Newcastle, New South Wales, Australia, 16-17 October, 2008
1-week workshop: Electrolyte Thermodynamics for faculty and students at University of Cape Town, South Africa, 7-11 April, 2008

Ioannis Tsivintzelis:
Poster presentation: Evaluation of the Non-Random Hydrogen Bonding (NRHB) Theory and the simplified Perturbed-Chain-Statistical Associating Fluid Theory (sPC-SAFT), I. Tsivintzelis, A. Grenner, I. Economou, C. Panayiotou, G. Kontogeorgis, Proceedings of the 23rd European Symposium on Applied Thermodynamics (ESAT), Cannes, France, 29 May to 1 June, 2008

Wei Yan:
Poster presentation: Measurement and Modelling of CO_2 Solubility in Brine and CO_2-Saturated Brine Density at High Pressures, Wei Yan, Shengli Huang, and Erling H. Stenby, SPE Applied Technology Workshop, Dubrovnik, Croatia, May 19-22, 2008.
Oral presentation: The Influence of CO_2 Solubility in Brine on CO_2 Flooding Simulation, Wei Yan and Erling H. Stenby, the 29th Annual Workshop and Symposium on IEA Collaborative Project on EOR, Beijing, China, November 3-5, 2008.

Master Thesis 2008

David Bøgh "Using spectroscopy data for developing association equations of state"

Casper Hadsbjerg Sørensen "Thermodynamic Modelling of Hydrocarbon Mixtures with the PC-SAFT Model"

Shengli Huang "Measurements and Modelling of CO_2 Solubility in Water and CO_2 – saturated Water Density at High Pressures"

Rama Krishna Raju Jampana "Experimental Studies of CO_2 Injection for Enhanced Oil Recovery"

Julie Jannerup, "Hydrodemetallization in Vacuum Gas Oils"

Asger Lindholdt "Thermodynamic Modelling of H_2S Solubility in Salt Solutions"

Maria Christine Malmos "Water Borne Wood Stains for Exterior Wood"

Vickram Mangru "Modelling of liquid-liquid equilibria of polymer solutions with the PC-SAFT equation of state"

Kenneth Ndumbe Ngale, "Transport in Tight Gas Reservoir"

Vasu Neela "Refrigeration Plants using Carbon Dioxide as Refrigerant: Permeability of Carbon Dioxide in Polymers used as Packing and Sealing Materials"

Saddia Qayyum, "Ion-exchange and rever sed phase chromatography"

Muhammad Riaz, "Design and Analysis of Extractive Separation Processes using Ionic Liquids"

Sara Sandersen, "Absorption Processes for CO_2 Capture"

Elham Sharifi, "Surfactants for Removal of Particle Contamination in Liquid CO_2 – Cleaning/ Extraction of Silicone Rubber"

Peter Christian Vestager Tybjerg , "Distribution of Polar Inhibitors in Oil-Water Mixtures"

IVC-SEP Publications 2008

SEP 0801
"Quality by design – Thermodynamic Modelling of Chromatographic Separation of Proteins"
Jørgen M. Mollerup, Thomas Budde Hansen, Steffen Kidal, and Arne Staby
(Journal of Chromatography A, 1177 (2008) 200-206)

SEP 0802
"Modeling Systems Containing Alkanolamines with the CPA Equation of State"
Ane S. Avlund, Georgios M. Kontogeorgis, and Michael L. Michelsen
(Industrial & Engineering Chemistry Research, 47(19) (2008) 7441-7446)

SEP 0803
"Fractional Flow Model for Suspension Transport in Porous Media (for Petroleum and Environmental Engineering)
Pavel Bedrikovetsky and Alexander Shapiro
(Oral presentation at the 10th World Filtration Congress, Leipzig, Germany, 14-18 April, 2008)

SEP 0804
"Phase Equilibrium Modelling for Mixtures with Acetic Acid using an Association Equation of State"
Núria Muro-Suñe, Georgios M. Kontogeorgis, Nicolas von Solms, and Michael L. Michelsen
(Industrial & Engineering Chemistry Research,47 (2008) 5660-5668)

SEP 0805
"Modelling of Phase Equilibria of Surfactant Mixtures using an Association Model"
Nuno M. F. Garrido, Georgios K. Folas and Georgios M. Kontogeorgis
(Fluid Phase Equilibria, 273 (1-2) (2008) 11-20)

SEP 0806
"Challenges in teaching "Colloid and Surface Chemistry" – A Danish Experience"
Georgios M. Kontogeorgis, and Martin E. Vigild
(Accepted by Chemical Engineering Education)

SEP 0807
"Multi-Scale Modeling of Structure, Dynamic and Thermodynamic Properties of Imidazolium-Based Ionic Liquids: Ab Initio DFT Calculations, Molecular Simulation and Equation of State Predictions"
I. G. Economou, E. K. Karakatsani, G. -E. Logotheti, J. Ramos, and A. Vanin
Oil & Gas Science and Technology, 63(3) (2008) 283-293)

SEP 0808
"Hydrolysis of Cellulose Using Mono-Component Enzymes Shows Synergy during Hydrolysis of Phosphoric Acid Swollen Cellulose (PASC), but Competition on Avicel"
Natalija Andersen, Katja S. Johansen, Michael L. Michelsen, Erling H. Stenby, Kristian B.R.M. Krogh, and Lisbeth Olsson

Photo: Mikkel Adsbøl

...IVC-SEP Publications 2008

(Enzyme and Microbial Technology, 42 (2008) 362-370)

SEP 0809
"Random-Walk Description of Suspension Transport in Porous Media"
Pavel Bedrikovetsky, and Alexander Shapiro
(Submitted for presentation at ICTAM 2008)

SEP 0810
"Modeling the Solid-Liquid Equilibrium in Pharmaceutical-Solvent Mixtures: Systems with Complex Hydrogen Bonding Behavior"
Ioannis Tsivintzelis, Ioannis G. Economou, and Georgios K. Kontogeorgis
(AIChE Journal, 55(3) (2009) 756-770)

SEP 0811
"Modeling Adsorption of Liquid Mixtures on Porous Materials"
Matias A. Monsalvo and Alexander A. Shapiro
(Journal of Colloid and Interface Science, 333(1) (2009) 310-316)

SEP 0812
"Refrigeration Plants Using Carbon Dioxide as Refrigerant: Measuring and Modelling the Solubility, Diffusivity and Permeability of Carbon Dioxide in Polymers Used as Packing and Sealing Materials"
Nicolas von Solms, and Vasu Neela
(Submitted to Journal of Heat Transfer Engineering"

SEP 0813
"Elliptic Random-Walk Equation for Suspension and Tracer Transport in Porous Media"
A.A. Shapiro, and P.G. Bedrikovetsky
(Physica A, 387 (2008) 5963-5978)

SEP 0814
"The Chilled Ammonia Process - Evaluation of the Energy Requirements"
Philip Loldrup Fosbøl, Erling H. Stenby, and Kaj Thomsen
(Internal Report)

SEP 0815
"Chilled Ammonia Process for CO_2 Capture"
Victor Darde, Kaj Thomsen, and Erling H. Stenby
(Internal Report)

SEP 0816
"Modelling the Phase Behavior in Mixtures of Pharmaceuticals with Liquid or Supercritical Solvents"
Ioannis Tsivintzelis, Ioannis G. Economou, and Georgios K. Kontogeorgis
(Journal of Physical Chemistry B, 113(18) (2009) 6446-6458)

SEP 0817
"A Review of the Thermodynamics of Protein Association to Ligands, Protein Adsorption, and Adsorption Isotherms"
Jørgen M. Mollerup
(Chem. Eng. Technol, 31(6) (2008) 864-874)

SEP 0818
"Study of High-Pressure Adsorption from Supercritical Fluids by the Potential Theory"
Matias A. Monslvo, and Alexander A. Shapiro
(Submitted to Fluid Phase Equilibria)

SEP 0819
"Analysis and Applications of a Group Contribution sPC-SAFT Equation of State"
Amra Tihic, Nicolas von Solms, Michael L. Michelsen, Georgios M. Kontogeorgis, and

Leonidas Constantinou
(Accepted by Fluid Phase Equilibria"

SEP 0820
"Application of sPC-SAFT and Group Contribution sPC-SAFT to Polymer Systems – Capabilities and Limitations"
Amra Tihic, Nicolas von Solms, Michael L. Michelsen, Georgios M. Kontogeorgis, and Leonidas Constantinou
(Accepted by Fluid Phase Equilibria"

SEP 0821
"Thermodynamics of Triethylene Glycol and Tetraethylene Glycol Containing Systems Described by the CPA Equation of State"
Martin Breil, Georgios M. Kontogeorgis
(Published online on Chemistry Research (in Press))

SEP 0822
"Modeling of Biopharmaceutical Processes: II Process Chromatography Unit Operation"
Oliver Kaltenbrunner, Justin McCue, Philip Engel, Jørgen Mollerup, and Anurag S. Rathore
(BioPharm International, 21(8) (2008) 28)

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(Presented at GHGT9, Washington, November 200)

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Wei Yan, and Erling H. Stenby
(Presented at the International Energy Agency (IEA) 29th Annual Workshop & Symposium , Beijing, China, November 3-5, 2008)

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