DTU

Annual Report 2007

IVC-SEP

Center for Phase Equilibria
and Separation Processes

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and Biochemical Engineering**

Technical University of Denmark

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IVC-SEP Annual Report 2007

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Allan Klo /StatoilHydro

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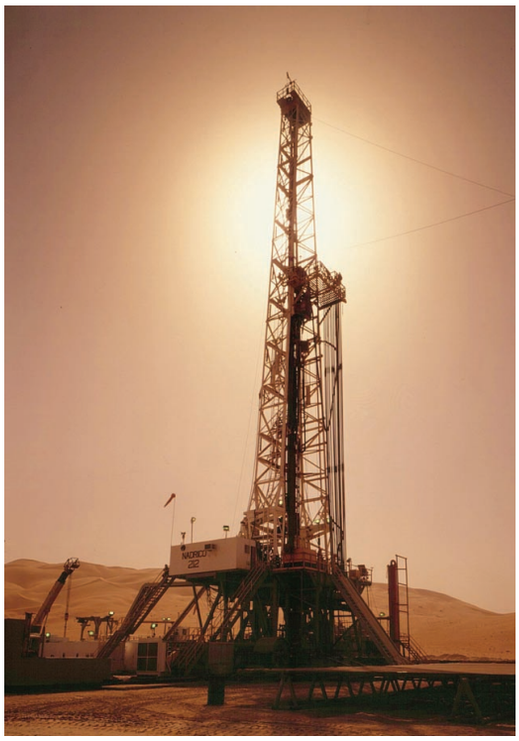

Longevity over political correctness

IVC-SEP may not always appear as the trendiest research group. We use the interest from our 25 member companies as a key indicator for importance

This IVC-SEP Annual Report is made to give you an overview of the centre activities during 2007. Selected projects are described in some detail as illustrations of our way of working on topics of relevance to the society often in collaboration with industry.

Applied thermodynamics is an important ingredient in most innovative products and processes. Thus our expertise can be utilized in many different businesses involving technology and production sciences.

The space of application of our experimental, theoretical, and computational skills covers the treatment of fly ash from biomass, advanced oil recovery methods, fundamental understanding of flow and transport in porous media in general, the behaviour of gas hydrates and their inhibitors, refinery processes, improving methods for to capture CO_2 and then storing it in geological structures, as well as many other subjects.

Some topics get more political attention than others but to a large extend we use the interest from our 25 member companies as an indicator for the importance of a given subject. This means that we may not always appear as the trendiest and politically correct research group. We believe that the longevity of this group and its success is based on a will and ability to move at the right moment and in the right direction based on our core competencies.

Should you have comments or questions after reading this report I will appreciate if you will contact me. Feed back, discussions, and challenges are important for our continuous development.

I hope you will find the report interesting and relevant.

Professor Erling Stenby,
Director of IVC-SEP

A more detailed summary of 2007 events to be found at page 19.

Erling Stenby
Director of IVC-SEP, professor
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IVC-SEP Konsortium:

StatoilHydro • Maersk Oil • Haldor Topsøe • BP • Linde • Eni • Total DONG Energy • Shell • OMV • IFP Chevron • Kommunekemi • BR • SQM • RWE • Akzo Nobel • Schlumberger • ExxonMobil • Vattenfall • Welltec • Saudi Aramco • Sasol • Novo Nordisk

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.

The Saudi Aramco Ras Tanura Refinery. Photo: Saudi Aramco

We welcome...

Saudi Aramco

One of the world's largest energy corporations has joined the IVC-SEP Consortium.

Saudi Aramco has 52,000 employees, 259.9 billion barrels of recoverable crude oil and condensate reserves and 248.5 trillion cubic feet of gas reserves. Not to mention an annual crude oil production of 3.25 billion barrels and 3.00 trillion cubic feet of annual gas production.

It is hard not to be impressed by the key figures (all figures are 2006) behind Saudi Aramco. Thus the inclusion of the corporation in IVC-SEP's Consortium constitutes a further strengthening of the centre's desired role as a partner to leading chemical, biochemical and energy companies worldwide.

Amongst the main focus areas of interest to Saudi Aramco we expect to see the fast and robust phase equilibrium calculations by Michael L. Michelsen and the development of thermodynamic models for the future. Also IVC-SEP research within EOR and history matching will be fields of mutual interest.

Sasol

Headquartered in Johannesburg, South Africa, Sasol is a World leader in coal-to-liquid and one of the top companies in gas-to-liquid.

Sasol was established in 1950 by the South African government to manufacture fuels and chemicals from indigenous raw materials. The company has developed world-leading technology for commercial production of synthetic fuels and chemicals from low-grade coal as well as the conversion of natural gas to environment-friendly fuels and chemicals.

A workforce of 30,000 is engaged in exploration, mining, science, technology R & D and business development.

Novo Nordisk

Novo Nordisk is a health care company and a world leader in diabetes health care. While IVC-SEP has traditionally been associated with the energy sector, we see the inclusion of a health care corporation in the IVC-SEP Consortium as an exiting new development.

Recent research has shown that a number of IVC-SEP strongholds such as simulation of separation processes may be of significance to pharmaceutics. An example of a relevant technology is chromatographic separation and purification of therapeutic proteins.

Novo Nordisk has the broadest diabetes product portfolio in the industry. In addition, Novo Nordisk has a leading position within areas such as haemostasis management, growth hormone therapy and hormone replacement therapy.

With headquarters in Denmark, Novo Nordisk employs approximately 23,600 full-time employees in 79 countries, and markets its products in 179 countries.

Cubic Equations - with a Plus

The use of a range of oil recovery related chemicals has prompted development of additional chemical theory. StatoilHydro is one of the companies utilizing the CPA (Cubic Plus Association) method

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.

Traditionally cubic equations of state (EOS) have been applied to describe phase equelibria 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.

»Within the oil industry cubic equations of state are in high standing. Fortunately one does not have to disregard them all together provided that one includes an additional element which explains the influence of other chemicals involved«, reader Georgios M. Kontogeorgis, IVC-SEP, explains.

Used in everyday problem solving

This adjusted model is called CPA - Cubic Plus Association. 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

Georgios Kontogeorgis
Reader
gk@kt.dtu.dk

Photo: Trym Ivar Bergsmo / StatoilHydro

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.

»Efficient and environmentally careful use of chemicals is crucial in oil and gas production. Through the fruitful cooperation with IVC-SEP we have gained first-hand access to the CPA model. Often the model has proven more accurate compared to the equations of state we have been using traditionally«, dr. Even Solbraa, Discipline Advisor for Gas Quality at StatoilHydro, states.

»Often the CPA model has proven more accurate compared to the equations of state we have been using traditionally«

Dr. Even Solbraa, Discipline Advisor for Gas Quality at StatoilHydro

»At StatoilHydro we use the CPA 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«, Even Solbraa adds.

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.

In the future CPA will be still more relevant, Even Solbraa predicts:

»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. In this respect our cooperation with the strong and recognized research environment at IVC-SEP is important«.

Photo: Allan Klo / StatoilHydro

They make use of CPA

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 me thanol and glycols, high pressure applications as well as phase equilibria for mixtures with other chemicals e.g. acetic acid. Current members are StatoilHydro, Total, BP and Maersk Oil.

StatoilHydro:

The world's third-largest net seller of crude oil and one of the world's largest gas suppliers. The company was established on October 1st 2007 following the merger between Statoil and Hydro's oil and gas activities. StatoilHydro has 31,000 employees in 40 countries. Production is averaging over 1.7 million barrels of oil equivalent per day. The company is the world's largest operator of deepwater fields.

Total:

The world's fourth largest integrated listed oil and gas company. The company, headquartered in France, has 95,000 employees, operations in more than 130 countries and exploration and production in 42 countries. Proved reserves amount to 11.1 billion barrels of oil equivalent as of December 31, 2006. Production is 2.36 million of oil equivalent per day.

"Maersk Oil appreciate the long standing cooperation with the IVC-SEP research group, particularly within the areas of applied thermodynamics and modelling of petroleum reservoir fluids and enhanced recovery methods.

Franz Willum Sørensen,
Intl. Production Development, Maersk Oil

Bio ethanol – a new frontier

The CPA model has relevance for all compounds involving hydrogen bonds. Associate professor Georgios M. Kontogeorgis, IVC-SEP, expects ethanol to become a major focus during the years to come:

»Worldwide the use of bio ethanol as gasoline additive is rising. In contrast to oil and gasoline ethanol is a hydrophilic compound. This creates a risk that the gasoline-ethanol mixture will attract water leading to phase separation. This is a question one needs to deal with – both at the refineries and in the engine of the individual vehicle«.

Another example of compounds containing hydrogen bonds is organic acids used for multiple purposes in the chemical and petrochemical industry. Again CPA is an appropriate tool.

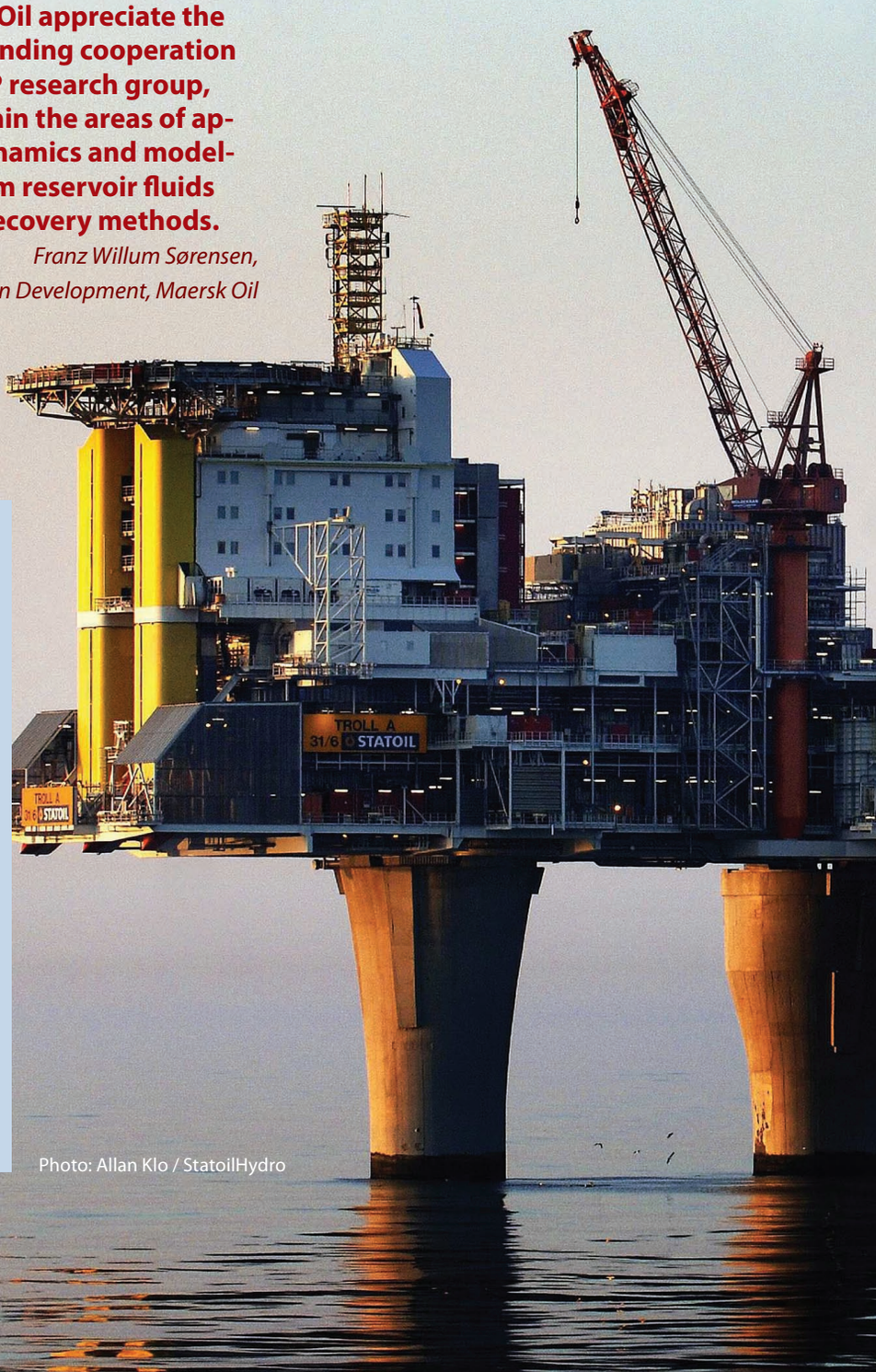
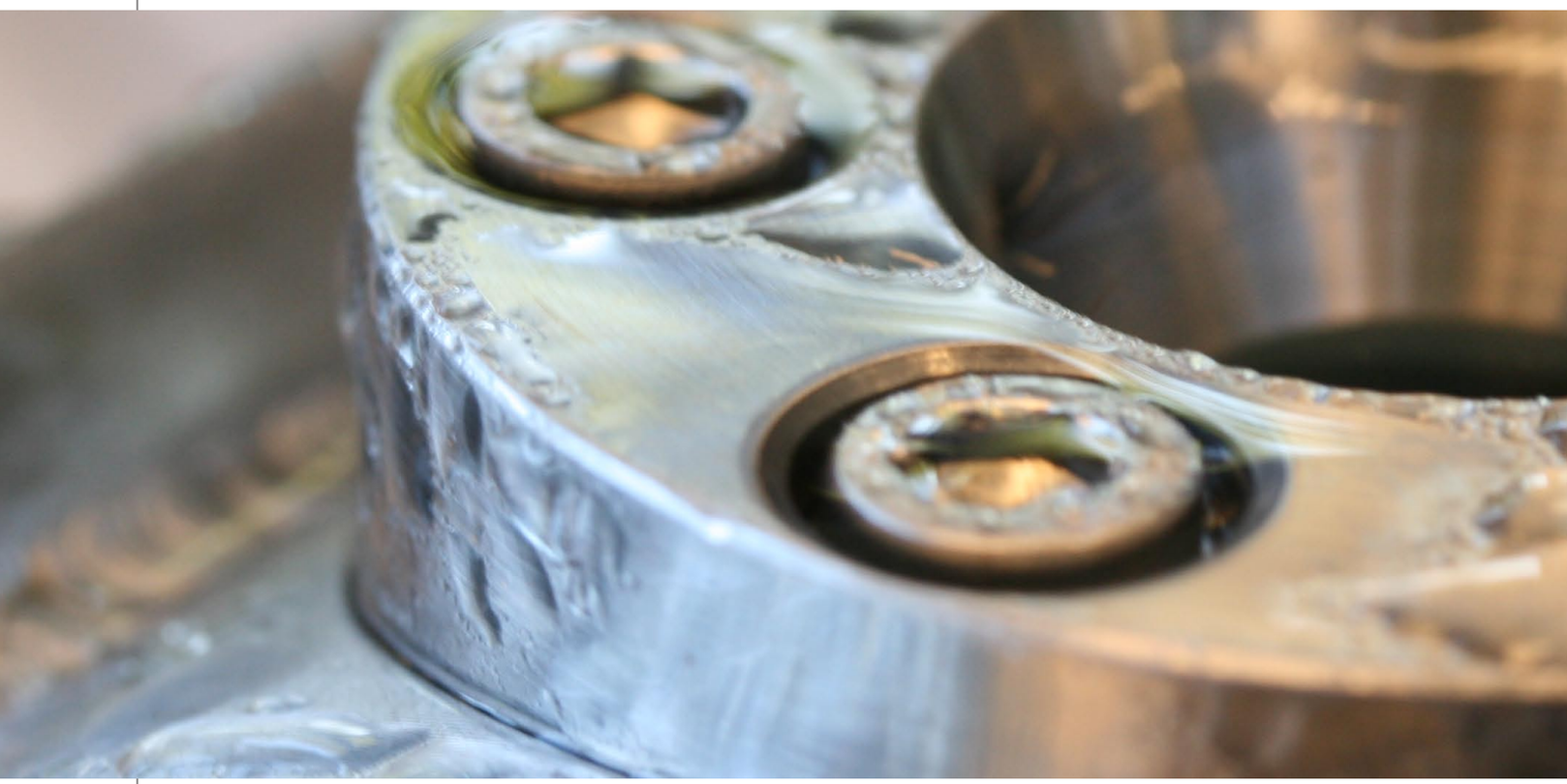


Photo: Allan Klo / StatoilHydro

BP:
One of the world's largest energy companies, providing its customers with fuel for transport, energy for heat and light, retail services and petrochemicals products for everyday items. Proven reserves equal 17.7 billion barrels of oil and gas equivalent. The number of employees by December 2006 was 97,000. BP operates 18 refineries and carry out exploration in 26 countries.

Maersk Oil:
An international oil and gas company operating an oil production of more than 600,000 barrels per day and a gas production of up to some 1,000 million cubic feet per day. The company has a net production equity 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.



Future Recovery under Cold Conditions

Small amounts of polymers added with the right timing might replace large quantities of gas hydrate inhibitors which are today required under recovery at Northern locations. So far the research is still at a theoretical stage.

As much as 40 % concentration of gas hydrate inhibitors may be seen in the fluid phase under recovery and transportation of oil and gas where hydrate-forming conditions are present. Fortunately the inhibitors are regained later in the process, but a certain loss is inevitable and the very handling of the large volume of inhibitors is associated with huge economical costs.

»Searching for alternative ways of preventing the formation of gas hydrates is surely worth considering«, associate professor Nicolas von Solms, IVC-SEP, states.

He and associate professor Kaj Thomsen are supervising a PhD study by Lars Jensen aiming just at examining alternative ways of inhibiting gas hydrate formation.

Influence the kinetics

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. As a result large quantities of inhibitors, primarily methanol and ethylene glycol, are utilized.

Nicolas von Solms,
Associate Professor
nvs@kt.dtu.dk

Because the polymers only act as catalyst you can do with small amounts compared to the inhibitors in use today. We see this as exciting.

Nicolas von Solms, associate professor, IVC-SEP

Photo: Christian Carlsson

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. Recovery under cold conditions presents high risk of hydrate formation. 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.

»Certain polymers have proven able to influence the kinetics of the process. They function as a reversed catalyst preventing the formation of hydrates. The effect is only temporary but if it is applied with the right timing – at the point where hydrate formation conditions would otherwise have been in place – these substances may be able to do the job. And because the polymers only act as catalyst you can do with small amounts compared to the inhibitors in use today. We see this as exiting«, Nicolas von Solms explains.

Given the economic potential one might think oil companies would already be lining up to take part in this field of research. However this has not been the case - yet.

»The most promising polymers investigated so far have not been sufficiently environmentally friendly. A certain amount of output to the marine environment is inevitable. We need to find polymers with a structure similar to those already proven efficient but with the extra quality of being biodegradable and environmentally acceptable in general«, Nicolas von Solms concludes.

Besides polymers acting as kinetic gas hydrate inhibitors a number of other alternative ways of preventing the growth or agglomeration of hydrates are under investigation.■

Moving from Low to Ultra Low Sulphur Diesel

Catalysts from Haldor Topsøe A/S already meet the toughest demands for diesel desulphurization. Still the company is looking for ways to improve the process

One of the major "engines" for the sale of catalysts for the refineries is environmental demands on diesel. A growing number of countries have demands for ultra low sulphur diesel (ULSD).

»We already market catalysts meeting the EU demand of maximum 10 ppm sulphur – which is the toughest demand in the World. Still we are striving to improve our catalysts further. Both in order to adapt to future demands and to maintain our leading market edge«, Kim G. Knudsen, head of refinery catalyst research at Haldor Topsøe A/S, says.

The World's sulphur emissions are already dramatically reduced. Even small amounts of sulphur in diesel will however disturb the catalyst responsible for reducing nitrogen-oxides from the exhaust gas. In other words: in order to reduce the emissions of nitrogen-oxides one needs to have ultra low sulphur content.

An additional goal is to obtain the lowest possible output of small particles which are a major health issue. As one would understand this sums up to a complicated chemical cocktail. The challenge is to balance the different goals in a way resulting in the lowest possible overall pollution.

A multi-phase system

Desulphurization is done through hydro treating. A mixture of liquids (primarily oil) and gas (primarily hydrogen) trickle downwards through a porous catalyst in a reactor. The result is sulphur bound to hydrogen in the form of H_2S.

The system involves three phases. Besides the oil and gas phases a solid phase is involved – the catalyst itself. In order to optimize the overall process one needs to understand and determine the phase equilibria involved.

At Haldor Topsøe A/S roughly fifty man years are spent on research in the field. These efforts are supplemented with projects in cooperation with IVC-SEP and other academic institutions.

"We do have in-depth understanding of the details in the many processes involved. The scientific scope which we share with IVC-SEP is to unite the details in large scale summations".

Kim G. Knudsen, head of refinery catalyst research at Haldor Topsøe A/S

»IVC-SEP has a high level of expertise in describing multi-phase system equilibria«, Kim G. Knudsen says.

Besides the main process one needs to understand a large number of side reactions, he stresses:

»Oil consists of several million subcomponents – this does complicate things. One just cannot do calculations including all subcomponents. Our answer is to group the subcomponents. We develop such a

Photo: Lars Poulsen, PolFoto

The Topsøe Group – Haldor Topsøe A/S of Denmark and its subsidiary companies is devoted to research and development in heterogeneous catalysis, production and sale of catalysts, and engineering and construction of catalytic units. The company has a permanent staff of about 1,400.
www.topsoe.com

model in cooperation with IVC-SEP«.

At IVC-SEP this project is carried out by PhD student Rasmus Boesen with associate professor Nicolas von Solms as supervisor and reader Michael Michelsen as co-supervisor.

Large scale summations

The theoretical understanding of the thermodynamics and matter transport involved is also within the scope of the efforts of the group at IVC-SEP.

»The thermodynamics and matter transport are important when one is to optimize the process. It all boils down to how fast the individual molecules will be able to migrate into the catalyst pellet«, says Kim G. Knudsen and sums up:

»At Haldor Topsøe A/S we do have in-depth understanding of the details in the many processes involved. The scientific scope which we share with IVC-SEP is to unite the details in large scale summations. Even being the Worlds leading ULSD catalyst suppliers we still want to improve!« ■

Desulphurization through hydro treating
A hydro treating unit is best described as a trickle-bed reactor, where liquid and gas flow co-currently down through the reactor, and where the liquid trickles from pellet to pellet and the gas forms a continuous phase.

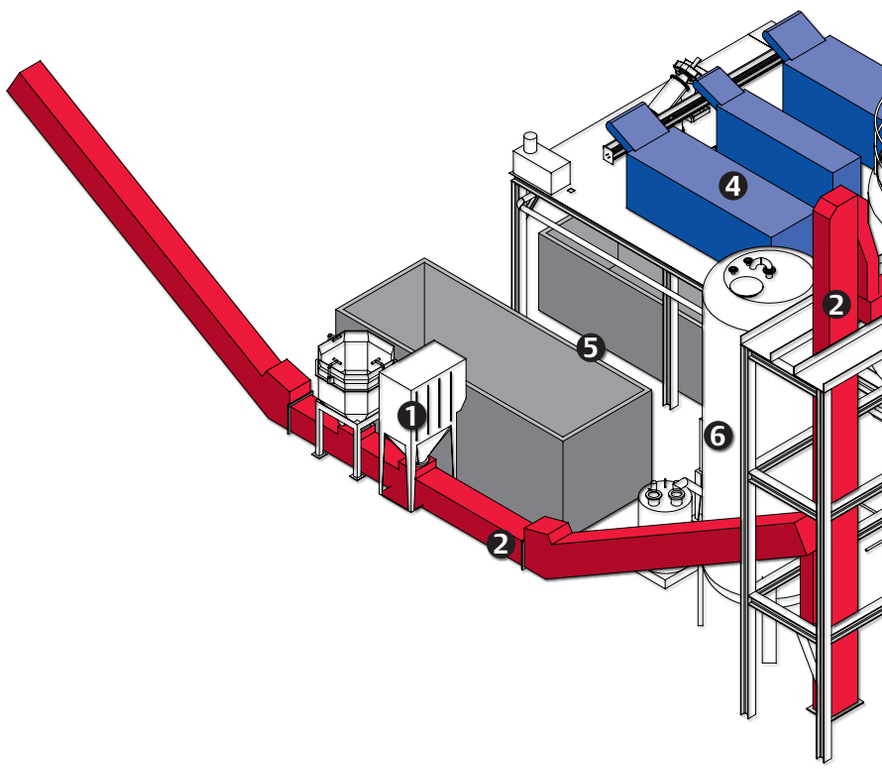
Demands in Sweden and California started off development

The efforts by Haldor Topsøe A/S within ULSD started in the first half of the 1990'ies. At that time Sweden and California chose to put demands on the content of aromatic compounds in diesel. It was realized that in order to limit the content of aromatic compounds one would need to minimize the sulphur content.

In spite of the potential market being rather limited the Danish company got down to work and actually succeed in limiting the sulphur content to just a few ppm. Haldor Topsøe A/S has been the Worlds leading supplier of ULSD catalysts ever since.

Today the EU has a demand for 10 ppm sulphur in diesel while the US has a 15 ppm demand.

Putting Ashes from Straw to Use as Fertilizer



Cadmium removal turns a waste problem into a product of value to farmers

Complete utilization of ashes from straw burnt at the power plants has still not been achieved.

»But I guess 99.6 % is not that bad after all«, Olof Malmros, Kommunekemi, says smilingly.

The high degree of utilization is expected to become reality by the end of 2008 as an existing production facility will then be modified for the purpose.

A yearly total of 10,000 tonnes of fly ash from straw is produced in Denmark. The ashes are rich in nutrients, first of all salts of potassium, and were previously used as agricultural fertilizers. However problems with heavy metals, mainly cadmium, have led to a stop for this application. This problem is solved by a new wet chemical process developed at Kommunekemi.

You may say the solution addresses two issues at the same time. A product useful to farmers is produced while at the same time a waste problem is solved. Or as Olof Malmros puts it:

»This development is driven by a dual purpose. We benefit the environment – and we make business«.

Dissolution properties are key focus

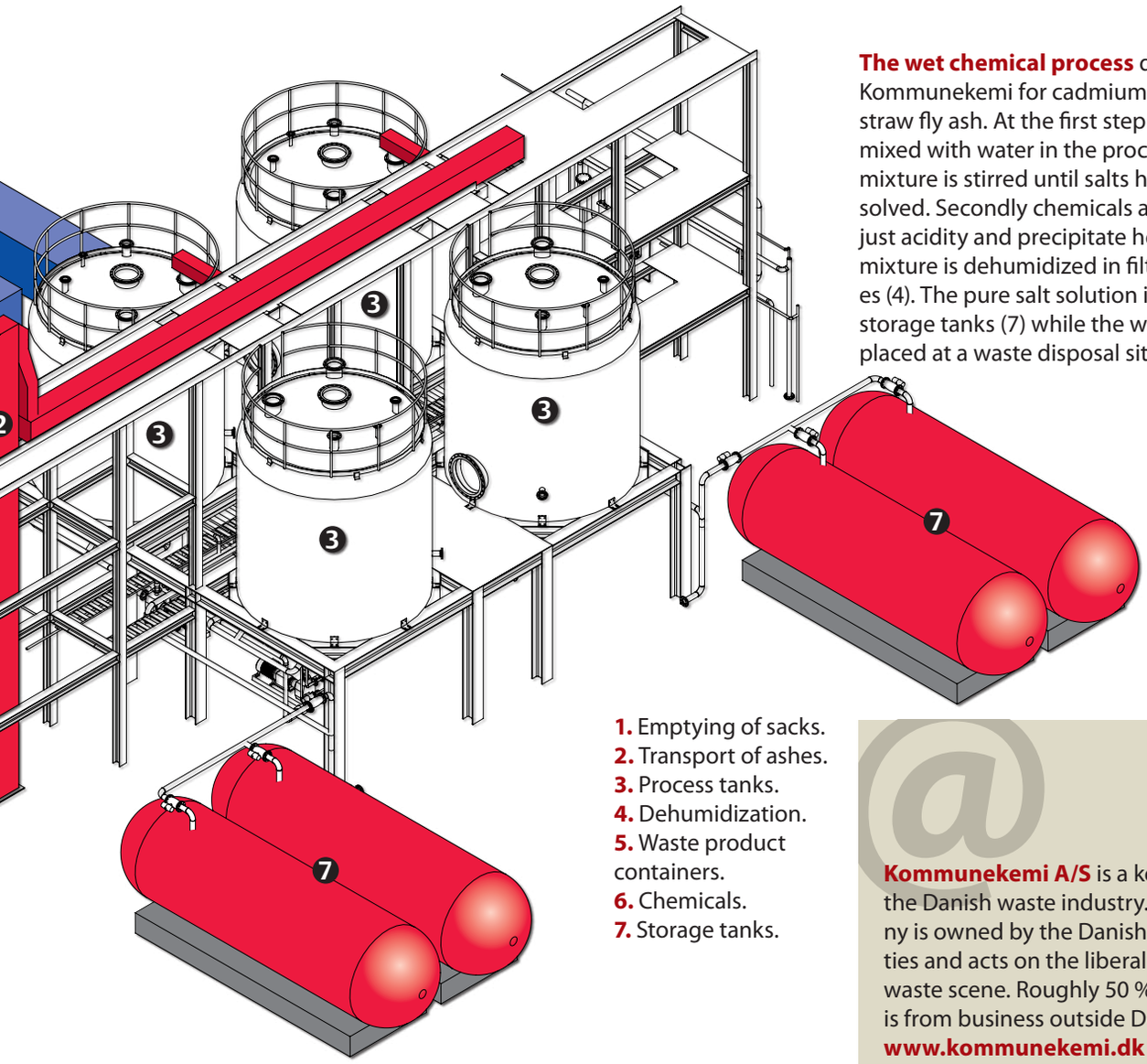
Kommunekemi is already producing a wet potassium chloride product sold to the Danish fertilizer industry.

»The cadmium removal technique was developed by us. IVC-SEP has assisted us in creating the theoretical framework for our trials«, says Olof Malmros adding:

»In a concentration of approximately 10 milligram per kilogram cadmium is definitely just a minor component in the straw ashes, but if you wish to remove it you need to understand

„The trials done here at Kommunekemi have been compared to theoretical results from IVC-SEP on an ongoing basis. This has enabled us to proceed significantly faster than we would otherwise have been able to.“

Olof Malmros, Kommunekemi



The wet chemical process developed at Kommunekemi for cadmium removal from straw fly ash. At the first step the ashes are mixed with water in the process tanks (3). The mixture is stirred until salts have been dissolved. Secondly chemicals are added to adjust acidity and precipitate heavy metals. The mixture is dehumidized in filters and presses (4). The pure salt solution is pumped to storage tanks (7) while the waste product is placed at a waste disposal site.

1. Emptying of sacks.
2. Transport of ashes.
3. Process tanks.
4. Dehumidization.
5. Waste product containers.
6. Chemicals.
7. Storage tanks.

Kommunekemi A/S is a key operator in the Danish waste industry. The company is owned by the Danish municipalities and acts on the liberalized European waste scene. Roughly 50 % of turnover is from business outside Denmark.
www.kommunekemi.dk

the dissolution properties of the major components. For that purpose we make use of a theory developed by associate professor Kaj Thomsen at IVC-SEP«.

Besides 50 % potassium chloride the straw ashes also contain 30 % potassium sulphate which has been placed at a waste disposal site so far. This is a real pity as potassium sulphate has at least double value as fertilizer compared to potassium chloride.

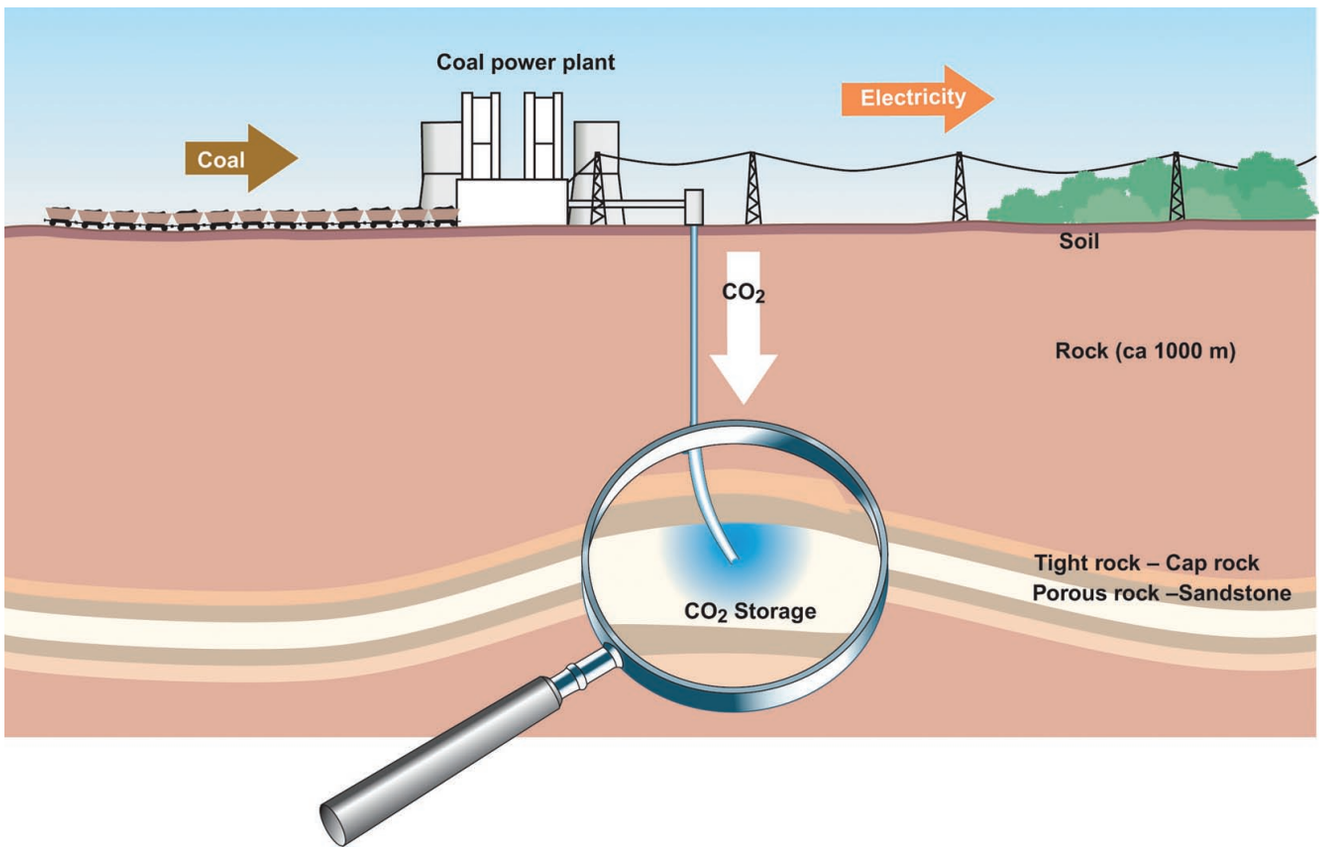
Ongoing relation

The wish for utilizing potassium sulphate was one on the reasons why Kommunekemi entered into cooperation with Kaj Thomsen and joined the IVC-SEP Consortium.

»The trials done here at Kommunekemi have been compared to theoretical results from IVC-SEP on an ongoing basis. This has enabled us to proceed significantly faster than we would otherwise have been able to", Olof Malmros says.

The production facility at Kommunekemi has a yearly capacity of 25,000 tonnes of agricultural waste products.

Besides ashes from straw the technique may be relevant to other types of ashes resulting from energy production by burning other types of biomass. ■



Carbon Capture from Theory to Practise

Carbon Capture and Storage (CCS) is a key technology in the attempt to limit global warming. IVC-SEP offers its partners "the full package" of disciplines involved in both carbon capture and storage. Source: Vattenfall

Energy corporations Vattenfall and DONG Energy are frontrunners when it comes to carbon capture and storage (CCS)

Ever more often CCS, Carbon Capture and Storage, is mentioned as one of the key technologies needed to limit global warming. Several IVC-SEP industrial consortium members are active in CCS research and development.

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 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«.

Non-carbon electricity

At the Schwarze Pumpe coal fired power plant in Germany Vattenfall is already building 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. Besides the expenses of the equipment itself one will have to accept a loss of energy related to capture and storage processes. My best estimate would be the electrical energy production efficiency of the power plants dropping from the present about 45 % down to about 35 %«.

»But then again: renewable energy is expensive as well. In my view CCS electricity should be compared to other types of non-carbon emitting electricity. In a direct comparison with offshore wind turbines and photo voltaic cells CCS may prove most economical. Finally it will be crucial to reach a popular consensus regarding carbon storage«.

Danish pilot plant

DONG Energy is another CCS frontrunner. Two years ago the company 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, NH3). 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.

DONG Energy does have thoughts on ways to improve energy efficiency.

»We are looking at other types of amine solvents just as we are looking at the possibility of replacing the amine solution with a mixture of ammonia and water. The IVC-SEP scientists are assisting us by working out process models"« Willy van Well says.

Besides these possible techniques various

"Carbon capture has entered the agenda of energy policy. The level of activity is so high that failure to achieve major progress in one or more CCS technologies would seem unlikely.

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

Strong commitment in Norway

At the Mongstad refinery in Norway a demonstration plan capturing CO_2 from the flue gas of a gas fired power plant is under construction.

Statoil, Vattenfall and DONG Energy are partners in the first stages of the project. IVC-SEP follows the project closely through the three energy corporations all of which are members of the IVC-SEP industry consortium.

»We are confident that our knowledge will prove to be useful to the project«, professor Erling Stenby, head of IVC-SEP, says.

DONG Energy was founded in 2006 as a result of a merger involving six Danish energy companies – DONG, Elsam, Energi E2, Nesa, Copenhagen Energy's power activities and Frederiksberg Forsyning. By the end of 2006 DONG Energy employed 4,585. The company is active in power generation, oil & gas exploration & production and in distribution. The focus area is the Northern European market where electricity, gas and related products are sold.
www.dong.dk

Vattenfall is Europe's fourth largest generator of electricity and the largest producer of heat. Consolidated sales in 2006 amounted to SEK 145,815 million. Operations today are conducted in Sweden, Denmark, Finland, Germany and Poland. Vattenfall works in all parts of the electricity value chain: generation, transmission, distribution and sales. Vatttenfall also conducts energy trading and lignite mining, and produces, distributes and sells heat. The Group has slightly more than 32,000 employees. The parent company, Vattenfall AB, is 100 % owned by the Swedish state.
www.vattenfall.dk

Schwarze Pumpe coal fired power plant in Germany where Vattenfall is building a pilot plant. Photo: Vattenfall

other CO_2 capture concepts are under development.

»The EU has initiated a lot of activity. It is a running train and now is the time to be on it. At DONG Energy we see the research in the field at DTU as exciting and contribute economically to various projects. At this point it is still too early to say which CO_2 capture technique will prove best«, according to Willy van Well.

At Vattenfall Hakon Mosbech agrees:

»One thing I do dare to predict is significant progress in one or more of the technologies in the near future. If you go back just 5-6 years CCS was not taken all that seriously. Worldwide you'd have less than 1,000 people doing research in the field. With CCS entering the agenda of energy policy this has changed dramatically. The level of activity is so high that failure to achieve major progress would seem unlikely«. ■

Tickets booked in due time

Director of IVC-SEP, professor Erling Stenby, underlines that the centre did book tickets for the running train in due time:

»CCS covers a number of issues. First of all capture but also storage. Putting the captured CO_2 to use for Enhanced Oil Recovery (EOR) is again an independent discipline. At IVC-SEP we do have expertise in all three fields. This allows us to offer our partners »the full package« of disciplines involved. I am pleased to be able to say we already have a strong CCS research environment in place. We are strongly committed to becoming one of the internationally leading CCS centres«.

Currently IVC-SEP has two Post Docs and two PhD students working full time on CCS. Additionally two PhD students are expected to start early 2008. ■

"It is a running train and now is the time to be on it. At DONG Energy we see the research in the field at DTU as exciting and contribute economically to various projects.

Willy van Well, coordinator of CO_2 capture technology development at DONG Energy

Reaching a High Level of Activity

Erling Stenby
Director of IVC-SEP,
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2007 was a year dominated by global shortage of skilled staff. Still IVC-SEP was able to attract the talents we need. We expect the very high level of activity reached to continue in the coming years

The IVC-SEP Annual Report 2007 summarizes the highlights of the past year and presents the potential and ideas for future development of our group.

On 30 May 2007 it was once again time for the annual Discussion Meeting of IVC-SEP. Believe or not this was the 28th consecutive Discussion Meeting and attendance has never been higher. Among other highlights we enjoyed 4 industrial presentations from member companies.

The IVC-SEP Consortium is as old as the Discussion Meetings and here we see the same positive development. We have welcomed the following companies this year: Sasol, Saudi Aramco and Novo Nordisk. This confirms to us that our research is still of high quality and relevance.

Besides our current members we are in constant dialogue with many non-member companies who take interest in our know-how and research. We discuss collaboration and topics of mutual interest. When this does not always lead to a real collaboration and a new member in the Consortium it usually means that we could not agree on terms and conditions.

There is an increasing pressure on academia to work closer with the industry. Unfortunately this may lead to discussions over commercial rights, confidentiality, exclusivity, time tables, and deliverables. If a company does not see a value in having close links to an information, knowledge and research center such as IVC-SEP where competitors can even meet on neutral ground and benefit from state-of-the-art research and expertise they normally do not join. In IVC-SEP we are convinced that we have the member companies that we should have.

Competing for talent

The global shortage of skilled staff has led to an increasing interest from member companies to support our research. We really appreciate these contributions. However IVC-SEP is not a commercial entity. Therefore we do not strive to maximize our economic profit. Our goal is to maximize production of high quality research and education. Quality should stay at the highest international level. The amount of work that we can do is limited by three key factors:

- 1.Faculty members for research, innovation, supervision and management.
- 2.Talented candidates for PhD and Post Doc positions
- 3.Funding for projects and long term investments

We have managed to maintain a good balance between these three factors for many years. The limiting factor has most often been the funding and occasionally finding the right PhD student at the right moment.

Today we have two challenges linked to the same reason namely the increasing competition for talent world wide. One challenge is the increasing interest from industry for funding smaller to medium size projects which are often addressing short term problems. This requires much attention from Faculty members and increases the administrative overhead.

To limit this burden we also seek to initiate larger projects and JIPs such as CHIGP in order to make efficient use of our resources. The second challenge is that increased activity requires more PhD students and Post Docs at a time where the job market is booming. Until now we have managed to meet this challenge

and we expect to be able to do so in the future.

During late 2006 and in 2007 we have initiated a number of new projects (the man power listed here relates to IVC-SEP staff only):

- CO_2 for Enhanced Oil Recovery 2007-2009. Collaboration with DONG Energy, Environment & Resources (DTU), the Geological Survey of Denmark and Greenland, and Geotechnical Institute. Funded by the Danish National Advanced Technology Foundation and DONG Energy. 1 PhD student + 1 Post Doc
- LUWS – Liquefaction in Unseparated Well Streams 2008-2010. Collaboration with Institute for Energy Technology in Norway and Statoil. Funded by the Norwegian Research Council. 1 PhD student
- Simulating Reactive Transport in Enhanced Oil Recovery 2006-2010. DTU PhD Scholarship. 1 PhD student
- 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 2007-2009 (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. With the commitment from most and maybe all of the previous participants which were: Statoil, BP, Total, and Maersk Oil. We also hope to have new companies joining soon. 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. The project is further more strengthened by a PhD scholarship from DTU. 2 PhD students + 1 Post Doc
- 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 6 PhD students and 2 Post Docs involved. Maersk Oil has joined as the first industrial sponsor and other member companies are invited to join. The project is a collaboration

The 2007 version of the annual IVC-SEP Discussion Meeing held at LO-skolen in Elsinore May 30th May to 1 June was the 28th consecutive event of its kind. Attendance has never been higher. Among other highlights were 4 industrial presentations by member companies.

with two DTU departments (DTU Mechanical Engineering and DTU Informatics) and the independent technology company GEO, specializing in geotechnical problems.

The last major theme is "CO_2 Capture and Storage". In addition to our ongoing capture and EOR activities we have recently worked hard on the chilled ammonia process. There are several challenges in simulating all the currently considered capture processes. We now have 5 coworkers in this area and will expand CCS activities during 2008. Again we welcome collaboration and input from member companies.

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

Courses fully booked

At the end of this report you will find an overview of the 47 manuscripts produced by the IVC-SEP coworkers during 2007. Members of the IVC-SEP Consortium can download 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.

The IVC-SEP Summer School 2007 focused on "Petroleum Reservoir Fluids". It took place in August and was very well attended by PhD students and industrial participants from many countries.

In January 2008 Michael L. Michelsen and Jørgen M. Mollerup will once again give their highly regarded course on "Thermodynamic Models: Theory and Computational Aspects". The course was quickly fully booked even though we have accepted 27 participants. Several participants come from our member companies. At the same time the second edition of the book by Michelsen and Mollerup from 2004 is released. The course will be given again in January 2009.

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. ■

Photo: Christian Carlsson

Two Issues Addressed in One Go

At one of the company's production sites in The North Sea DONG Energy is currently considering a pilot project aimed at utilizing t from thermal power plants for Enhanced Oil Recovery (EOR)

Any oil company would like to enhance the amount of oil recovered from its production sites – Enhanced Oil Recovery (EOR). At the same time use of fossil fuels results in carbon emissions contributing to global warming. Why not address both issues in one go?

»The world faces two major challenges in respect to energy policy. One is security in supply, the other is climate protection. A¡s carbon dioxide may act as a solvent it might be used in EOR. This is a way of dealing with both capital issues at the same time«, says Charles Nielsen, head of R&D at DONG Energy.

»You might also turn the question around and ask: if we are to store carbon dioxide in the ground in any case – why not use it to enhance oil production?«

The average degree of oil recovery in the Danish part of The North Sea is about 25 %. In other words 75 % is left. A one per cent increase would represent oil worth 10 billion USD.

From on-shore to off-shore

When carbon dioxide is pumped into an oil field with adequate pressure it will mix with oil. The result is a thinning of the 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.

The method is highly sensitive to application of the correct pressure. If the pressure is too low carbon dioxide and oil will not mix completely. This has a number of undesired implications. However to just apply a high level of pressure is not a good solution. This will create risk of causing damage to the reservoir and at the same time the economical consequences are negative as one will be using excessively large and costly equipment.

»Unfortunately all experience with this kind of EOR comes from on-shore and involve different types of geological structures compared to those known in The North Sea. In other words a major piece of R&D is needed before one can think of putting the idea into practise«, Charles Nielsen says.

Still DONG Energy remains determined to take the method further. Among the partners in this quest are university researchers, including IVC-SEP.

»From the moment we decide to move ahead we tend to focus on the practical side of things. It is important to have an academic support base«, Charles Nielsen says adding:

»One interesting issue is the immediate events. How will the equilibria between carbon dioxide, water, gas and oil look? Another issue that we need to look at is the long term implications. How will the process affect the geological structures at the site?«

Like squeezing a sponge

You need to take into account both the nature of the given geological structure and the type of oil in it. Some types of oil are more suited for carbon dioxide EOR than others. In other words we cannot use general guidelines. You have to evaluate from case to case whether a given production field is a candidate for carbon dioxide EOR«, professor Erling Stenby, director of IVC-SEP, comments.

»At IVC-SEP we have worked on EOR by

"From the moment we decide to move ahead we tend to focus on the practical side of things. It is important to have an academic support base.

Charles Nielsen, head of R&D at DONG Energy for Gas Quality at StatoilHydro

DONG Energy - Exploration

40 % of activity (measured by EBITDA) in DONG Energy is oil & gas exploration. Revenues from oil & gas exploration and production totalled 5,556 million DKK in 2006. The exploration and production activities are carried out in Danish, Norwegian, UK and Faroese waters. DONG Energy also operates Denmark's only oil pipeline, which takes the oil from the North Sea to the Fredericia oil terminal.

Photo: DONG Energy/Lars Sundshøj

gas injection including carbon dioxide for many years. Our thermodynamic tools are state of the art and we know where the need for further research is«.

The method 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. To sum up: subsidence may be positive, but only if it takes place in a controlled manner«, Erling Stenby explains.

An academic support base

At one of the company's production sites in The North Sea DONG Energy is currently considering a pilot project aimed at utilizing carbon dioxide for EOR. IVC-SEP and Institute for Environment and Resources at DTU constitute the academic support base for the project together with The Geological Survey of Denmark and Greenland (GEUS) and Danish Geotechnical Institute

»First of all we expect scientists to point to which parameters we need to measure in order to obtain grounds for estimating the long run consequences for geological structures«, says Charles Nielsen, DONG Energy.

»Secondly we expect scientists to assure that we are getting the sufficient amount of data in order for us to calculate whether it will be possible to make carbon dioxide EOR economically feasible«. ■

Quality by Design

A PAT tool for thermodynamic modelling of chromatographic separations of proteins

Chromatographic separation and purification of biological products are of singular importance to the pharmaceutical health care industries that produce therapeutic proteins because this is the only separation process that can deliver a high purity product. Hence, one reason for the ubiquity of chromatographic steps in preparative protein purification is that they provide a relatively efficient means to meet manufacturing goals.

Development of a recovery and purification scheme for a therapeutic protein has to progress rapidly in order to enable the production of the active pharmaceutical ingredient for the clinical trials. Therefore, it is mandatory to develop a robust purification process at an early stage of the project that delivers a high purity product of a predefined quality. This means that the separation process developed at the laboratory scale should be suitable for scale-up.

An important tool for verifying the usefulness of a given chromatographic separation process is computer simulations. Besides saving the costs and manpower needed for numerous tests the possibility of doing simulations will also provide the manufacturer with a PAT tool that can supplement the experimental documentation requested by the Agency to get registration of a new drug. A manufacturer will need to provide a high degree of assurance that a specific process will consistently produce a product meeting predetermined specifications and quality attributes consistent with the current drug quality system and compliant with the requirements of the regulatory bodies.

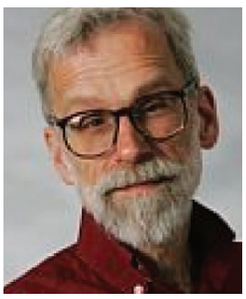
An important analytical tool

Regulatory issues are crucial for development and production of pharmaceuticals. All products must pass adequate controlled clinical trials to prove efficacy and document the benefit to risk ratio. The clinical studies supporting registration include; Phase 1: Preliminary studies most often in healthy volunteers; Phase 2: Studies to establish clinical proof of concept; Phase 3: Studies conducted to establish sufficient documentation to support safety, efficacy and marketing claims.

By phase 1 clinical trials it is requested to provide the Agency with a process flow sheet including a short description of the production process and the assays used in the quality control of the active pharmaceutical ingredient. It is possible to make changes in the process after the start of phase 2 but too many amendments to the process provided by phase 1 may require an extension of the clinical tests to provide the sufficient validation of the amendments.

»Thus by ensuring the right process layout at an early stage the manufacturer will be able to save a great deal of costs including those associated with additional clinical testing. One may call this idea quality by design«, explains reader Jørgen Mollerup, IVC-SEP.

In this context PAT (Process Analytical Technology) becomes an important tool to organise, to understand and supplement the available experimental information. Generally, the term analytical in PAT is viewed broadly to include physical, mathematical, chemical and microbiological tools, and risk assessment conducted in an integrated manner. An appropriate combination of some, or all, of these tools may be applicable to a single unit operation, or to an entire manufacturing process and its quality assurance system to acquire information to facilitate an improved theoretical and experimental process understanding and improve experience. Process innovation is provided by combining experimental data, general process understanding, theory



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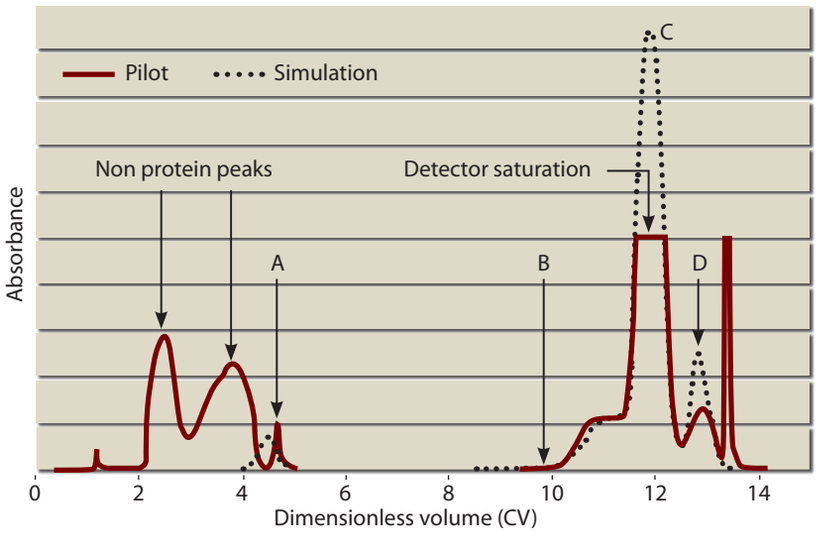
”Thus by ensuring the right process layout at an early stage the manufacturer will be able to save a great deal of costs including those associated with additional clinical testing. One may call this idea quality by design.

Jørgen Mollerup. docent at DTU



The figure shows a comparison of a simulated and an experimental run in the pilot plant. The yield and purity of the product C are shown in the table.

The data collected from a comparison of the pilot plant data and the simulated data shown in the figure. The purity is shown as the concentrations of the contaminants A, B, and D.

	A [%]	B [%]	D [%]	Yield	The collected volume relative to the column volume
Starting material	7.6	2.0	9.0		
Pilot plant	0.0	0.1	1.0	84	1.1
Simulation	0.0	0.0	1.1	84	1.1

References:
Jørgen M. Mollerup, Thomas Budde Hansen, Steffen Kidal, Lars Sejergaard, Arne Staby. Development, modelling, optimisation and scale-up of chromatographic purification of a therapeutic protein. Fluid Phase Equilibria 261 (2007) 133–139

Quality by design - Thermodynamic modelling of chromatographic separation of proteins. Jørgen M. Mollerup, Thomas B Hansen, Steffen Kidal, Arne Staby. Journal of Chromatography A. In press.

of processes, and modelling to develop a rational approach to the development, validation, scale-up and approval of a new process.

A robust purification process

A chromatographic separation is a robust purification process. It is developed through a number of steps including high-throughput screening of different resins and techniques to select appropriate candidates for a detailed investigation of the retention behaviour and capacity studies in dependence of the process variables that comprise particle size, pH, type and concentration of salt, solvents, additives, flow rate, gradient shape and length, and temperature. The solid phase in a chromatographic column can be rigid or soft and the expressions adsorbent, medium, gel, matrix, resin and beads are in common usage.

The chromatographic resins cover a variety of functions and applications from capture over intermediate purification to final purification in a down-stream process. Resins used for a capture step are characterised by having a fairly large particle size and a high binding capacity that may concentrate the target protein by removal of water and reduction of host cell proteins while avoiding clogging of the column by fermentation products. Intermediate purification is employed for further removal of host cell proteins and some product related impurities. Resins for final purification steps are typically characterised by having a small particle size with high selectivity.

A rational process development scheme

The ion-exchangers cover a broad range of commercially available backbone matrix chemistries including agarose, acrylic polymers, methacrylate, polystyrene-divinyl benzene, silica, as well as ceramics. The selection of the right chromatographic method and process variables is often performed by combining past experience with the trial and error method and this requires a lot of experiments.

To ensure a rational process development scheme, combining experiments, chromatographic theory, and modelling provide a tool that reduces the required number of experiments substantially because the model parameters can be estimated from a very limited number of experiments. The figure shows a comparison of a run in the pilot plant and the simulated result, and the table shows the yield and the purity of the experimental and the simulated run. Simulations can be used to develop the process and to investigate the influence of critical process parameters on the separation efficacy and the robustness of the process as regards product yield and purity. Once an optimal and robust process has been developed and scaled-up, it must be verified experimentally to validate the result of the model prediction and to satisfy the requirements of the regtulatory bodies. ■

CO_2 Capture from Coal Fired Power Plants

Jostein Gabrielsen

Jostein Gabrielsen
PhD
Today works with
Haldor Topsoe A/S

he purpose of the thesis is to contribute to the development of efficient carbon dioxide capture technology useful for coal fired power plants. This has been done through modelling, theoretical and experimental work.

The thesis introduces various post combustion CO_2 capture technologies with an emphasis on reactive absorption using aqueous solutions of alkanol amines.

A rate-based absorber model is developed and presented along with the theory needed to develop a model for reactive absorption in a packed column.

A thermodynamic model capable of presenting the CO_2 solubility in aqueous solutions containing one alkanol amine (MEA, DEA, MDEA, AMP, Piperazine) and one mixture (Piperazine/MDEA) is presented. From the proposed model an expression for the heat of absorption of CO_2 in the same solutions is derived. The model is developed specifically to be valid under conditions encountered during CO_2 capture from coal fired power plants.

Experimental data and calculated values of the rate constants for the reaction of CO_2 with AMP in an aqueous solution using a string of discs absorber are presented. Furthermore, experiments were carried out in order to define the mass-transfer area of the string of discs desorber.

Detailed experimental pilot plant data at 11 different process conditions are presented for a complete CO_2 absorption/desorption unit in an integrated laboratory pilot plant using an aqueous AMP solution. Temperature profiles over the absorber and desorber are included in the experimental data.

Validation of the proposed rate-based absorber model is carried out for CO_2 absorption using solutions of both MEA and AMP. This is done using both experimental data generated in this study and experimental data found in the literature. ■

Photo: Christian Carlsson

Development of an Equation of State for Solutions containing Electrolytes

Yi Lin

The thesis deals with equation of state (EOS) for aqueous electrolyte mixtures. Six electrolyte EOS' were developed from the residual Helmholtz free energy. Four out of the six electrolyte EOS' are selected for regression of ion-specific parameters of the test system consisting of six ions (Na+, Ca^{2+}, H+, Cl-, OH- SO_4^{2-}) and water. Both temperature independent and temperature dependent parameters have been obtained for the test system.

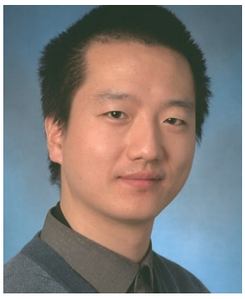
An introduction to the theories and models of electrolyte systems is given. The need for an electrolyte equation of state is stated.

Thermodynamic concepts pertinent to the rest of the thesis are derived or studied. The six electrolyte EOS' established in the work are presented. Mathematic aspects of developing electrolyte EOS' are dealt with. The vector analysis and calculus of multi-variable functions have been applied here to derive derivatives. The composition, temperature and volume derivatives of the Helmholtz free energy terms are deducted and presented in Appendixes. They are fundamental to the electrolyte EOS'.

Experimental density data collection for IVC-SEP electrolyte databank are dealt with and they are used for correlation of parameters for electrolyte EOS' in the later chapters. The IVC-SEP electrolyte databank is also briefly discussed.

A preliminary study of the six implemented electrolyte EOS' using salt-specific parameters for binary system is carried out. All electrolyte EOS' and their source codes are tested and checked thoroughly and programming errors are corrected. The comparison between EOS' and different terms are provided. Based on these studies four out of six EOS' are chosen for multi-component aqueous electrolyte systems at room temperature. The results are shown and temperature independent parameters are regressed. Phase diagrams for binary, ternary systems of ions are introduced. The abilities of electrolyte EOS' are illustrated and compared. A good representation of the experimental data is obtained.

Finally aqueous multi-component electrolyte systems at a wide temperature range is dealt with. Temperature dependent ion-specific parameters and their temperature dependence function are presented. The four electrolyte EOS' can represent phase diagrams of the test system at a wide temperature range. Model extrapolation with respect to temperature is not very satisfactory. ■



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Enzymatic Hydrolysis of Cellulose - Experimental and Modelling Studies

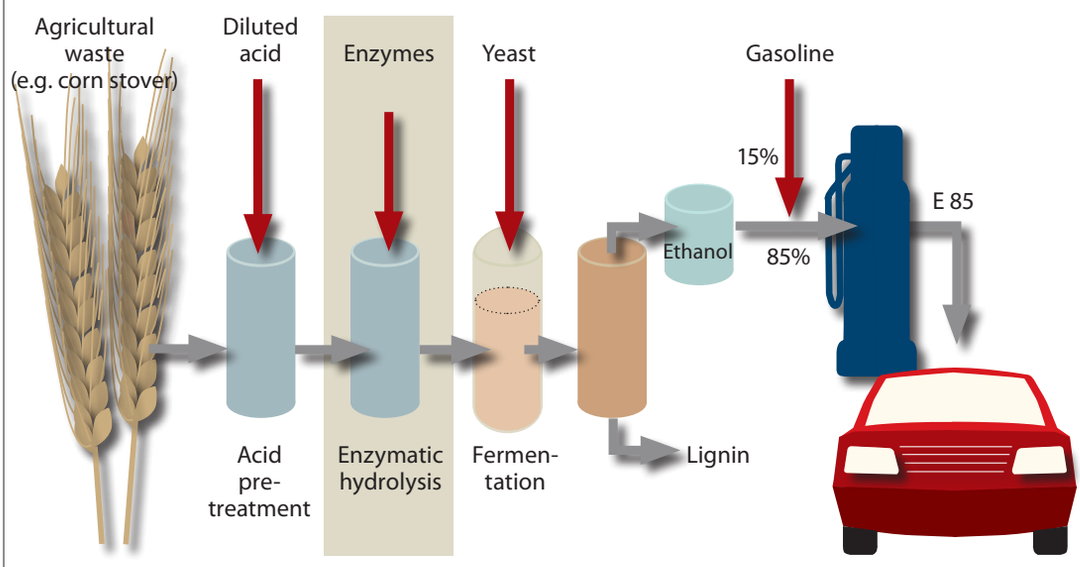
Natalija Andersen

The focus of the thesis is second-generation biofuel technology, and more precisely the process of enzymatic hydrolysis of cellulose. In general terms, the production of bioethanol from lignocellulose involves a degradation of the polymeric compounds, primarily cellulose and hemicellulose, to sugars, which are then fermented by microorganisms to ethanol. The process can be performed in a number of different ways.

The composition of lignocellulose (plant cell wall polysaccharides) is introduced and the characteristics of cellulose from plant materials (used in the industrial processes) and cellulose from model substrates, readily used in research, are discussed and compared. Cellulolytic enzymes and their main characteristics are introduced. One of the main characteristics of the cellulose hydrolysis process is the cooperative action, often designated synergy, of the different enzyme classes involved in the degradation process. Synergy is dependent on a variety of factors of which substrate characteristics play an important role. The cooperative action between the three enzyme classes (EG, CBH and BG) was investigated on two model cellulose substrates (Avivel and phosphoric acid swollen cellulose, PASC). Moreover, enzyme and substrate related factors affecting the hydrolysis, often represented by decrease of the hydrolysis rate in the later stage of the process, are discussed.

To better understand the fundamentals of this process, data obtained in the experimental studies were compared and evaluated against a mechanistic mathematical model describing the hydrolysis process. Additionally a novel approach based on application of the metabolic control analysis t heory was investigated as an alternative way of modelling, and, consequently, determining the most rate controlling step(s) / enzymes of the process. In general, mathematical modelling of the enzymatic hydrolysis process can offer increased understanding of the fundamentals of this process, and consequently lead to better choice of enzyme mixtures for hydrolysis. ■

BioCentrum DTU has hosted Natalija Andersen PhD study. Reader Michael Michelsen and professor Erling Stenby, both IVC-SEP, have been co-supervisors.



Natalija Andersen
PhD
Today works in
Novo Nordisk

Production of bioethanol from lignocellulose involves a degradation of the polymeric compounds, primarily cellulose and hemicellulose, to sugars, which are then fermented by microorganisms to ethanol. Mathematical modelling of the enzymatic hydrolysis process may offer increased understanding of the fundamentals of this process, and consequently lead to better choice of enzyme mixtures for hydrolysis.

To better understand the fundamentals of this process, data obtained in the experimental studies were compared and evaluated against a mechanistic mathematical model describing the hydrolysis process. Additionally a novel approach based on application of the metabolic control analysis t heory was investigated as an alternative way of modelling, and, consequently, determining the most rate controlling step(s) / enzymes of the process.

Research Funding in IVC-SEP

The research carried out in IVC-SEP is funded by grants from a number of public and private sponsors. In Denmark the PhD students study for a period of 3 years on top of their MSc degree. They are employees at normal salary and pension conditions. Thus a PhD project requires a secured funding of EUR 250,000 just for the student's salary, ordinary operational expenses, tuition and overhead. If equipment and technical assistance is needed this has to be added. This means that we need to raise a significant amount of money to maintain the current level of activity with more than 15 PhD students. Since our activities have grown over the latest decade we now also have a number of Post Doctoral fellows and Researchers in temporary positions. When we include our technical and administrative staff as well as our investments we come to a budget for 2007 of EUR 2.1 million.

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. ■

The main grants can be represented in the following manner:

Projects 2007 (kEUR)	
CHIGP	210
ADORE	80
MiMiCS	80
CO2 EOR	230
CCS	200
Gas Hydrates	170
PhD grants DTU	390
Other Private	570
Other Public	200
Total external funding	2130

Photo: Krydsfelt

Conference Contributions and Invited Speakers

Participants at The IVC-SEP PhD Summer School

Martin P. Breil - assistant professor

- Strategic Energy Research, 27 August 2007, Copenhagen, Oral presentation »Modelling of CO_2 Capture«, M.P. Breil, G.M. Kontogeorgis, and E.H. Stenby
- The European Congress of Chemical Engineering (ECCE6), Copenhagen 16-21 September, 2007, Oral presentation »Designing with CAPE-OPEN«, M.P. Breil, J. Gabrielsen, N. von Solms, G.M. ontogeorgis, and E.H. Stenby

Ioannis Economou – visiting professor

- 11th International Conference on Properties & Phase Equilibria for Product and Process Design, Hersonissos, Crete, Greece, 20 - 25 May 2007, Poster presentation »Atomistic Simulation of Silicon-Containing Elastomers: Force Field Development, Structure and Thermodynamic Properties of Polymer Melt and Solubility of n-Alkanes, n-Perfluoroalkanes, Noble and Light Gases«, Z.A. Makrodimitri, and I.G. Economou
- 11th International Conference on Properties & Phase Equilibria for Product and Process Design, Hersonissos, Crete, Greece, 20 - 25 May 2007, Poster presentation, »Calculation of the Effect of Macromolecular Architecture on Structure and Thermodynamic Properties of Linear - Tri-arm Polyethylene Blends from Monte Carlo Simulation«, A.N. Rissanou, L.D. Peristeras, and I.G. Economou
- 11th International Conference on Properties & Phase Equilibria for Product and Process Design, Hersonissos, Crete, Greece, 20 - 25 May 2007, Poster presentation »Prediction of Thermodynamic Properties and Phase Equilibria of Polar Multicomponent Mixtures from Perturbation Theory«, E.K. Karakatsani, and I.G. Economou
- 11th International Conference on Properties & Phase Equilibria for Product and Process Design, Hersonissos, Crete, Greece, 20 - 25 May 2007, Poster presentation »Experimental Measurements and Modeling using tPC-PSAFT of the Phase Behavior of the Ternary Ionic Liquid System CO_2 + water + [bmim] NO_3«, M.C. Kroon, E.K. Karakatsani, M. Montero, I.G. Economou, G.-J. Witkamp, and C.J. Peters
- The European Congress of Chemical Engineering (ECCE6), Copenhagen 16-21 September, 2007, Oral presentation »Evaluation of Statistical Mechanics-Based Equations of State for Complex Fluid Mixtures«, I.G. Economou, A. Grenner, I. Tsivintzelis, C. Panayiotou, and G.M. Kontogeorgis
- The European Congress of Chemical Engineering (ECCE6), Copenhagen 16-21 September, 2007, Oral presentation »Modeling of Ionic Liquid Binary and Ternary Mixture Phase Equilibria at Low and High Pressure With the tPC-PSAFT«, I.G. Economou, E.K. Karakatsani, M.C. Kroon, C.J. Peters and G.-J. Witkamp
- The European Congress of Chemical Engineering (ECCE6), Copenhagen 16-21 September, 2007, Oral presentation »Molecular Simulation and Macroscopic Modeling of Thermodynamic and Transport Properties of Silicon-Containing Rubbery Polymer - Solvent Mixtures«, I.G. Economou, Z.A. Makrodimitri, A. Tihic and G.M. Kontogeorgis
- Thermodynamics 2007, Paris, France, 26 - 28 September 2007, Oral presentation »Structure and Thermodynamic Properties of Poly(ethylene oxide) from Molecular Dynamics Simulations«, H. Leontiadou and I.G. Economou
- Thermodynamics 2007, Paris, France, 26 - 28 September 2007, Oral presentation »Molecular Modelling of 1-n-hexyl-3-methylimidazolium bis(trifluoromethanesulfonyl)imide Ionic Liquid«, G.-E. Logotheti, F.J. Ramos-Díaz, and I.G. Economou
- Department of Chemical Engineering, Technical University of Denmark, Lyngby, 24 January 2007, »Prediction of Structure and Physical Properties of Complex Fluids Using Molecular Simulation«. Invited.
- Department of Materials Science and Technology, University of Crete, Heraklion, Crete, Greece, 27 April 2007, »Structural and Physical Properties of Complex Fluids via Molecular Simulation Methods«. Invited.
- 2nd Innovative Modeling Technology Consortium Meeting and Seminar, National Technical University of Athens, Greece, 4 June 2007, »Materials Property Predictions Using Equation of State Theories«. Invited.

Corinne Eenschooten - industrial PhD student

- 8th Annual Meeting of the Skin Forum, 3-4 April 2007, School of Pharmacy, University of London, London, United KingdomPoster presentation: »Development of Colloidal Carriers from Modified Hyaluronic Acid«, Eenschooten C., Deli F., Guillaumie-Longin F., Kontogeorgis G.M., Stenby E.H., Schwach-Abdellaoui K., Gurny R.
- 7th International Conference on Hyaluronan, 22-27 April 2007, Charleston Francis Marion Hotel, Charleston, South Carolina, United States, Poster presentation: »Development of Colloidal Carriers from Modified Hyaluronic Acid«, Eenschooten C., Deli F., Guillaumie-Longin F., Kontogeorgis G.M., Stenby E.H., Schwach-Abdellaoui K., Gurny R.
- 21st Conference of the European Colloid and Interface Society, 10-14 September 2007, Geneva International Conference Center, Geneva, Switzerland. Poster presentation: »Development of Colloidal Carriers from a Novel Amphiphilic Hyaluronic Acid« Eenschooten C., Vaccaro A., Delie F., Guillaumie-Longin F., Kontogeorgis G.M., Stenby E.H., Schwach-Abdellaoui K., Borkovec M., Gurny R.

Philip Fosbøl - PhD student

- IVC-SEP Study trip, Statoil, Trondheim, Norway, 18 – 21 June, Oral presentation »Measurement and modelling of salt solubility in the mixed solvent CO_2-MEG-H_2O system«, Philip L. Fosbøl, Kaj Thomsen, and Erling H. Stenby
- NACEExpo 2007 konference, Nashville, TN, USA, 11 March, Poster presentation »Phase equilibria and CO_2 Corrosion - A new approach to corrosion modelling«, Philip L. Fosbøl, Kaj Thomsen, and Erling H. Stenby
- IVC-SEP Study trip, Trondheim, Norway, 18 – 21 June, Poster presentation »Phase equilibria and CO_2 Corrosion - A new approach to corrosion modelling«, Philip L. Fosbøl, Kaj Thomsen, and Erling H. Stenby
- European Congress of Chemical Engineering (ECCE-6), Copenhagen, 16-20 September 2007, Poster presentation »Phase equilibria and CO_2 Corrosion - A new approach to corrosion modelling«, Philip L. Fosbøl, Kaj Thomsen, and Erling H. Stenby
- Future Energy Research konference, RISØ, 9 October, Poster presentation »Phase equilibria and CO_2 Corrosion - A new approach to corrosion modelling«, Philip L. Fosbøl, Kaj Thomsen, and Erling H. Stenby

Lars Jensen - tPhD student

- Petroleum Technology Day, Technical University of Denmark, 28 March 2007, Oral presentation »Gas Hydrates- Formation and Inhibition«, Lars Jensen, Nicolas von Solms, and Kaj Thomsen
- IVC-SEP Study trip, Statoil, Trondheim, Norway, 18 – 21 June, Oral presentation »Research Activities on Gas Hydrates at IVC-SEP«, Lars Jensen, Nicolas von Solms, and Kaj Thomsen
- Aabenraa HTX, Roskilde gymnasium, Ørestads gymnastion, 25 – 28 September 2007, High school presentations during the Danish Science Festival, Oral presentation »Brændende snebolde«

Georgios Kontogeorgis - reader

- The European Congress of Chemical Engineering (ECCE6), Copenhagen 16-21 September, 2007, Oral presentation, »Modelling of associating mixtures for applications in the oil and gas and chemical industries«, G.M. Kontogeorgis, M.L. Michelsen, G. Folas, N. von Solms, and E.H. Stenby
- »Thermodynamics 2007, 26-28 September 2007, IFP – Rueil-Malmaison, France«, Oral presentation, »Solvation phenomena in association theories«, G.M. Kontogeorgis, F.K. Folas, N. Muro-Sune, F. Roca Leon, N. von Solms, M.L. Michelsen, and E.H.Stenby
- The 11th International Conference on Properties and Phase Equilibria for Product and Process Design (PPEPPD), 20-25 May, 2007, Hersonissos, Crete, Greece, Oral presentation, »Modelling of associating mixtures for applications in the oil & gas and chemical industries«, G.M. Kontogeorgis, G.K.Folas, N. Muro-Sune, N. von Solms, M.L.Michelsen, and E.H. Stenby

Participants at The IVC-SEP PhD Summer School

...Conference Contributions and Invited Speakers

Study trip to Norway, Statoil Trondheim

Morten Rode Kristensen - PhD student

- SPE Reservoir Simulation Symposium, Houston, Texas, USA, February 26-28, Poster presentation »Coupling Chemical Kinetics and Flashes in Reactive, Thermal and Compositional Reservoir Simulation«, SPE 106218, In Proceedings. Morten R. Kristensen, Margot G. Gerritsen, Per G. Thomsen, Michael L. Michelsen and Erling H. Stenby,
- 28th International Energy Agency Symposium on Enhanced Oil Recovery, Vedbæk, Denmark, September 4-7, 2007, Oral presentation »Integration of Chemical Reactions in Reservoir Simulation«, In proceedings, Morten R. Kristensen, Margot G. Gerritsen, Per G. Thomsen, Michael L. Michelsen and Erling H. Stenby,

Jørgen Mollerup - reader

- 5th HIC/RPC Bioseparation Conference, March 20-23, 2007, Interlaken, Switzerland, Oral presentation, »The thermodynamic principles of chromatography«
- PPEPPD 2007, Hersonissos, Crete, Greece, May 20-25, 2007, Oral presentation, »Recovery of Biological Products - Development, Modelling, Scale-up and Design of a Chromatographic Purification of a Therapeutic Protein«
- International Conference on Biopartitioning and Purification (BPP2007), Lisbon, Portugal, June 17 - 20, 2007, Poster presentations, »Ligand Binding I: Ion-Exchange Chromatography«, »Ligand Binding II: Hydrophobic Interaction Chromatography and Solubility« and »Ligand Binding III: Cooperativity«
- World Biopharm 2007, Bioseparation and Bioprocessing of Biological Products Queens' College, Cambridge, UK. 24-26, September, 2007, Oral presentation »Quality by design«

Matias Monsalvo - post doc

- Eleventh International Conference on Properties and Phase Equilibria (PPEPPD 2007), Hersonissos, Crete, Greece, May 20th - 25th, 2007, Poster, »Prediction of Adsorption from Liquid Mixtures in Microporous Media« Monsalvo M.A., Shapiro, A.A.
- European Congress of Chemical Engineering (ECCE6), Copenhagen, Denmark, September, 16th – 21st, 2007, Poster, »Prediction of Binary Adsorption Equilibria« Monsalvo M.A., Shapiro, A.A
- Future Energy Research Conference, RISØ, Roskilde, Denmark, October 9th, 2007, Poster presentation, »An Engineering Model for Adsorption of Gas and Liquid Mixtures on Microporous Solids« Monsalvo M.A., Shapiro, A.A.

Nicolas von Solms - associate professor

- 5th International Conference on Heat Transfer, Fluid Dynamics and Thermodynamics, July 1-4, 2007, Sun City, South Africa, Oral presentation »Gas-Polymer Interactions in Carbon Dioxide Refrigeration Plants«
- European Congress of Chemical Engineering (ECCE-6), 16-21 September, 2007, Copenhagen, Denmark, Oral presentation »How can spectroscopy help us to model hydrogen bonding fluids?«

Erling H. Stenby - professor

- 6 February, »Oil – plenty for this and the next generation« (in Danish), Sub soil Technology and Services, Offshore Center Denmark, Esbjerg, Denmark. Invited
- 1 March, »Denmark as an Oil Nation«, (in Danish), Jyske Bank's Energy Seminar, Copenhagen. Invited
- 28 March, »Recent Results from the Petroleum Engineering Research at IVC-SEP«, Petroleum Technology Day, Technical University of Denmark
- 6 June, »CO_2 Capture and Storage«, Siemens, Erlangen, Germany. Invited
- 18 – 21 June, »An Overview of IVC-SEP«, University of Bergen and Statoil Research Trondheim, IVC-SEP Study trip, Trondheim, Norway
- 6 August, Danish National Radio P1, 1 hour interview and discussion on the role of petroleum in the future. Invited
- 14 September, »CO_2 for EOR - Do's and Don'ts«, CO_2 Emissions Reductions, Marcus Evans Conference, Berlin. Invited
- 25-26 October, »Short Course on Phase Behavior of Petroleum Reservoir Fluids«, University of Bergen. Invited

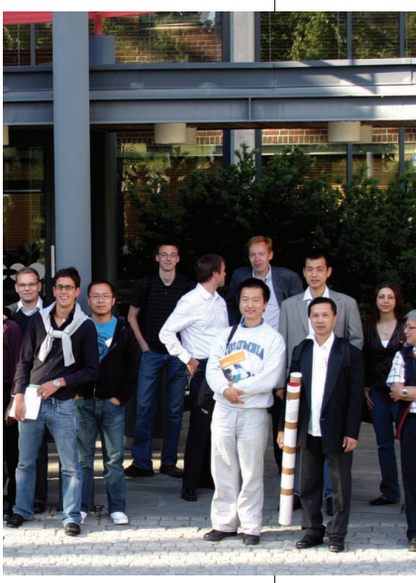
■ 23 November, »Petroleum Research at DTU – Challenges and Perspectives«, Offshore Soil Investigation Forum (OSIF), GEO, Kgs. Lyngby, Denmark. Invited
■ 29 November, Launch Ceremony of Center for International Business and Innovation (CIBI), »How to Collaborate with International Industry on Research and Innovation as Academic Researchers?«, Copenhagen Business School, Copenhagen. Invited

Amra Tihic - PhD student
■ Conference on Properties and Phase Equilibria for Product and Process Design (PPEPPD), 20-25 May, 2007, Hersonissos, Crete, Greece, Poster »Development of a Group Contribution Simplified PC-SAFT Equation of State«, Amra Tihic, Georgios M. Kontogeorgis, Nicolas von Solms, Michael L. Michelsen, and Leonidas Constantinou
■ European Congress of Chemical Engineering (ECCE-6), 16-21 September, 2007, Copenhagen, Denmark, Oral presentation »Development of a Group Contribution Simplified PC-SAFT Equation of State«, Amra Tihic, Georgios M. Kontogeorgis, Nicolas von Solms, Michael L. Michelsen, and Leonidas Constantinou
■ Thermodynamics 2007, 26-28 September, 2007, Rueil-Malmaison, France, Poster, »Development of a Group Contribution Simplified PC-SAFT Equation of State«, Amra Tihic, Georgios M. Kontogeorgis, Nicolas von Solms, Michael L. Michelsen, and Leonidas Constantinou

Kaj Thomsen - assiciate professor
■ The European Congress of Chemical Engineering (ECCE6), Copenhagen 16-21 September, 2007, Oral presentation, »Equation of State for Electrolyte Solutions«, Kaj Thomsen and Yi Lin

Yiannis Tsivintzelis - post doc
■ European Congress of Chemical Engineering (ECCE-6), Copenhagen, 16-20 September 2007, Poster presentation »Evaluation of Statistical Mechanics-Based Equations of State for Complex Fluid Mixtures« I.G. Economou, E.K. Karakatsani, A.Grenner, I. Tsivintzelis, C. Panayiotou. G.M. Kontogeorgis

Wei Yan - associate professor
■ SPE Annual Technical Conference and Exhibition, 11-14 November, Anaheim, CA, USA. Oral prese ttntation »Application of the CPA Equation of State to Reservoir Fluids in Presence of Water and Polar Chemicals«, W. Yan, G.M. Kontogeorgis, and E.H. Stenby



Study trip to Norway, Statoil Trondheim

Master Theses 2007

Lars Jensen »Gas Hydrates – Formation and Inhibition«

Christoffer Buhl Lund »Optimization of Sugar Yield in Sugar Production by using Organic Solvents to treat Molassis«

Rasmus Risum Boesen »Development of a Reactor Model for Trickle-Bed Hydro Desulfurization Units«

Ángel Llaneza Carceller »Osmotic Pressure of Proteins«

Jonas Lyberg Kofod »Modelling of Phase Equilibria for Mixtures of Relevance to the PTA Process«

Jakob Kristensen »Polymers in Refrigeration Plants with Carbon Dioxide as Cooling Substance«

Rasmus Lundsgaard »Migration of Phthalates from PVC«

Christopher Berglund »Injection of CO_2 in Calcareous Rocks with low Permeability – a Potential EOR Method«

Victor Camille Alfred Darde »Environmental Aspects of CO_2 Capture from Flue Gas«

Arlindo Mieiro »Determination of Solid-Liquid Equilibrium using Conductivity Measurements«

Nuno Garrido »Modeling of Complex Chemicals in Oil Industry with CPA«

Paula Marie Gilsenan »Chromatographic Scale-up Studies using Model Protein Systems«

Ane Søgaard Avlund »Octanol-Water Position Coefficients of Chemicals in Oil Industry«

Yassir I. Z. Ghiyati »Investigation of Recombination – Reaction of Olefins and Hydrogen Sulphide«

Steen Larsen »Production of Decadmiated Phosphate by Crystallization and Ion Exchange«

Dennis Setorwu Adrah »Modelling of Ethanol-Water-Gasoline Phase Equilibria with the CPA Equation of state«

Stine Bothmann Bergmann/Soniasara Yasin »Calculations of Phase Equilibria with Gas Hydrate Inhibitors with CPA«

Soniasara Yasin »Calculations of Phase Equilibria with Gas Hydrate Inhibitors using the CPA Model«

Michael Tvedebrink Jensen »Modellering of Wax Deposition in Pipes«

Rama Krishna Raju Jampana »Modellering and Simulation of Enhanced Oil Recovery by CO_2 Injection«

Elham Sharifi "Surfactants in Dry-cleaning of Silicone Rubber"

Ram Mohan Reddy Vempada »Sequestration of Carbon Dioxide in Aquifers«

Vasu Neela »Permeability of CO_2 in Polymers used in CO_2 Refrigeration Plants«

Kenneth Ngale Ndumbe »Transport in Tight Gas Reservoir«

IVC-SEP Publications 2007

Photo: Christian Carlsson

SEP 0701
»High-pressure Vapor-liquid Equilibria of Systems Containing Ethylene Glycol, Water and Methane. Experimental Measurements and Modeling«
■ Georgios K. Folas, Ole J. Berg, Even Solbraa, Arne O. Fredheim, Georgios K. Kontogeorgis, Michael L. Michelsen and Erling H. Stenby
(Fluid Phase Equilibria, 251 (2007) 52-58)

SEP 0702
»Data and Prediction of Water Content of High Pressure Nitrogen, Methane and Natural Gas«
■ Georgios K. Folas, Einar W. Froyna, Jørgen Løvland, Georgios M. Kontogeorgis and Even Solbraa(Fluid Phase Equilibria, 252 (2007) 162-174)

SEP 0703
»Use your own models in process simulation. CAPE-Open – an international standard«
■ Martin P. Breil, Georgios M. Kontogeorgis, Nicolas von Solms and Erling H. Stenby
(Accepted by Journal of Chemical Engineering)

SEP 0704
»Global Phase Equilibrium Calculatuins: Critical Lines, Critical End Points and Liquid-Liquid-Vapour Equilibrium in Binary Mixtures«
Martin Cismondi and Michael L. Michelsen
(Journal of Supercritical Fluids, 39 (3) (2007) 287-295)

SEP 0705
»Multi Component Equations of State for Electrolytes«
■ Yi Lin, Kaj Thomsen and Jean-Charles de Hemptinne
(AIChE Journal, 53(4) (2007) 989-1005)

SEP 0706
»Solubility of Gases and Solvents in Silicon Polymers: Molecular Simulation and Equation of State Modeling«
■ Ioannis Economou, Z.A. Makrodimitri, Georgios M. Kontogeorgis, Amra Tihic
(Journal of Molecular Simulation, 33 (2007) 851-860)

SEP 0707
»Calculation of the Effect of Macromolecular Architecture on Structure and Thermodynamic Properties of Linear – Tri-Arm Polyethylene Blends from Monte Carlo Simulation«
■ Anatassia n. Rissanou, loukas D. Peristeras and Ioannis G. Economou
(Polymer, 48 (2007) 3883-3892)

SEP 0708
»Application of the CPA Equation of State to Reservoir Fluids in Presence of Water and Polar Chemicals«
■ Wei Yan, Georgios M. Kontogeorgis and Erling H. Stenby
(Submitted to Journal of Petroleum Science and Engineering)

SEP 0709
»Application of PC-SAFT to Glycol Containing Systems – PC-SAFT Towards a Group Contribution Method«
■ Andreas Grenner, Georgios M. Kontogeorgis, Nicolas von Solms and Michael L. Michelsen
(Fluid Phase Equilibria, 261(1-2) (2007) 248-257)

SEP 0710
»Hybridization of the Probability Perturbation Method with Gradient Information«
■ Kent Johansen, Jef Caers, Satomi Suzuki
(Accepted by Journal of Computational Geosciences)

SEP 0711
»On the Estimation of Water Pure Compound Parameters in Association Theories«
■ A. Grenner, G. M. Kontogeorgis, M. L. Michelsen and G. K. Folas
(Molecular Physics, 105(13-14) (2007) 1737-1801)

SEP 0712
»Modeling Phase Equilibria of Alkanols with the Simplified PC-SAFT Equation of State and Generalized Pure Compound Parameters«
■ A. Grenner, G. .M. Kontogeorgis, N. v. Solms and M. L. Michelsen
(Fluid Phase Equilibria, 258(1) (2007) 83-94)

...IVC-SEP Publications 2007

Photo: Christian Carlsson

SEP 0713
»Modelling of Associating Mixtures for Applications in the Oil & Gas and Chemical Industries«
■ Georgios M. Kontogeorgis, Georgios K. Folas, Núria Muro-Suñe, Nicolas von Solms, Michael L. Michelsen and Erling H. Stenby
(Fluid Phase Equilibria, 261 (2007) 205-211)

SEP 0714
Letter to the editor. Comments on »Measurement and Modeling of the Solubility of Water in Supercritical Methane and Ethane from 310 to 477 K and Pressures from 3.4 to 110 MPa«
■ Georgios M. Kontogeorgis and Wei Yan
(Industrial and Engineering Chemistry Research, 46(12) (2007) 4347-4348)

SEP 0715
»Measurement and Modelling of Hydrogen Bonding in 1-alkanol + n-alkane Binary Mixtures«
■ Nicolas von Solms, Lars Jensen, Jonas L. Kofod, Micheal L. Michelsen and Georgios M. Kontogeorgis
(Fluid Phase Equilibria, 261(1-2) (2007) 272-280)

SEP 0716
»Experimental Validation of a Rate-based Model for CO_2 Capture Using an AMP Solution«
■ J. Gabrielsen, H. F. Svendsen, M. L. Michelsen, E. H. Stenby and G. M. Kontogeorgis
(Chem. Eng. Sci., 62 (2007) 2397-2413)

SEP 0717
»Experimental Investigation of Liquid Chromatography Columns by Means of Computed Tomography«
■ Dirk-Uwe Astrath, Florian Lottes, Duc Thoung Vu, Wolfgang Arlt, and Erling H. Stenby
(Adsorption, 13 (2007) 9-19)

SEP 0718
»Refrigeration Plants Using Carbon Dioxide as Refrigerant: Measuring and Modelling the Solubility and Diffusion of Carbon Dioxide in Polymers used as Sealing Materials«
■ Nicolas von Solms, and Jakob Kristensen
(Submitted to Journal of Heat Transfer Engineering)

SEP 0719
»Adsorption of Amylase Enzyme on Ultrafiltration Membranes«
■ Søren Prip Beier, Ann Dorrit Enevoldsen, Georgios M. Kontogeorgis, Ernst B. Hansen, and Gunnar Jonsson
(Langmuir, 23(18) (2007) 9341-9351)

SEP 0720
»The Hansen Solubility Parameters (HSP) in Thermodynamic Models for Polymer Solutions«
■ Georgios M. Kontogeorgis
(Chapter in the book »Hansen Solubility Parameters – A user´s handbook« by Charles Hansen, CRC Press, 2nd edition (In press))

SEP 0721
»A Splitting Technique for Analytical Modelling of Two Phase Multicomponent Flow in Porous Media«
■ A. P. Pires, P. G. Bedrikovetsky, and A. A. Shapiro
(Journal of Petroleum Science and Engineering, 51 (2006) 54-67)

SEP 0722
»Study of the Solubility of a Modified Bacillus licheniformis α-Amylase around the Isoelectric Point«
■ Cornelius Faber, Timothy J. hobley, Jørgen Mollerup, Owen R. T. Thomas, and Svend G. Kaasgaard
(J. Chem. Eng. Data, 52 (2007) 707-713)

SEP 0723
»Adhesion between coating layers based on epoxy and silicone"«
■ Jacob R. Svendsen, Georgios M. Kontogeorgis, Søren Kiil, Claus E. Weinell, and Martin Grønlund
(Journal of Colloid and Interface Science, 316 (2007) 678-686)

SEP 0724
»Coupling Chemical Kinetics and Flashes in Reactive, Thermal and Compositional Reservoir Simulation«
■ M. R. Kristensen, M. G. Gerritsen, P. G.

Thomsen, M. L. Michelsen, and E. H. Stenby (SPE 106218, In Proceedings of the SPE Reservoir Simulation Symposium, Houston, Texas, USA, February 26-28, 2007)

SEP 0725
»Gas Transport in Tight Porous Media. Gas Kinetic Approach«
■ A. A. Shapiro, and J. A. Wesselingh
(Accepted by Elsevier Chemical Engineering Journal)

SEP 0726
»Prediction of Adsorption from Liquid Mixtures in Microporous Media by the Potential Theorgy«
■ Matias A. Monsalvo, and Alexander A. Shapiro
(Fluid Phase Equilibria, 261 (2007) 292-299)

SEP 0727
»Influence of Structured Packing on Gas Holdup in a Three-Phase Bubble Column«
■ Matías Monsalvo, and Ursula Böhm
(Chemical Engineering Science, 62 (2007) 6595-6603)

SEP 0728
»High-pressure Viscosity Behavior of x 1,1,1,2-tetrafluoroethane (HFC-134a) + (1-x) Triethylene Glycol Dimethylether (TriEGDME) Mixtures: Measurements and Modeling«
■ Matías A. Monsalvo, Antoine Baylaucq, Sergio E. Quiñones-Cisneros, and Christian Boned
(Fluid Phase Equilibria, 247 (2006) 70-79)

SEP 0729
»Corrigendum to "High-pressure Viscosity Behavior of x 1,1,1,2-tetrafluoroethane (HFC-134a) + (1-x) Triethylene Glycol Dimethylether (TriEGDME) Mixtures: Measurements and Modeling« [Fluid Phase Equilibria 247 (2006) 70-79]"
■ Matías A. Monsalvo, Antoine Baylaucq, Sergio E. Quiñones-Cisneros, and Christian Boned
(Fluid Phase Equilibria, 258 (2007) 95-97)

SEP 0730
»Efficient Integration of Stiff Kinetics with Phase Change Detection for Reactive Reservoir Processes«
■ Morten R. Kristensen, Margot G. Gerritsen, Per G. Thomsen, Michael L. Michelsen, and Erling H. Stenby
(Transport in Porous Media, 69 (2007) 383-409)

SEP 0731
»A Predictive Group-Contribution Simplified PC-SAFT Equation of State: Application to Polymer Systems«
■ Amra Tihic, Georgios M. Kontogeorgis, Nicolas von Solms, and Michael L. Michelsen
(Accepted by Industrial & Engineering Chemistry Research)

SEP 0732
»Measurement and Modelling of the Mixed Solvent Electrolyte System Na_2CO_3-$NaHCO_3$-Mono Ethylene Glycol-Water«
■ Philip L. Fosbøl, Kaj Thomsen, and Erling H. Stenby
(Submitted to Industrial and Engineering Chemistry Research)

SEP 0733
»Predictions of Flavonoid Solubility in Ionic Liquids by COSMO-RS: Experimental Verification, Structural Elucidation, and Solvation Characterization«
■ Zheng Guo, Bena-Marie Lue, Kaj Thomsen, Anne Boye Strunge Meyer, and Xuebing Xu
(Green Chemistry, 9 (2007) 1362-1373)

SEP 0734
»A Review and Recommended Thermodynamic Properties of $FeCO_3$«
■ Philip L. Fosbøl, Kaj Thomsen, and Erling H. Stenby
(Submitted to Corrosion Engineering Science and Technology)

SEP 0735
»Automated Calculation of Complete Pxy and Txy Diagrams for Binary Systems«
■ Martín Cismondi, and Michael L. Michelsen
(Fluid Phase Equilibria, 259 (2007) 228-234)

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...IVC-SEP Publications 2007

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SEP 0736
»Evaluation of the Non-Random Hydrogen Bonding (NRHB) Theory and the Simplified Perturbed-Chain-Statistical Associating Fluid Theory (sPC-SAFT) 1. Vapor-Liquid Equilibria«
■ Andreas Grenner, Ioannis Tsivintzelis, Georgios M. Kontogeorgis, Ioannis G. Economou, and Costas Panayiotou
(Submitted to Industrial and Engineering Chemistry Research)

SEP 0737
»Evaluation of the Non-Random Hydrogen Bonding (NRHB) Theory and the Simplified Perturbed-Chain-Statistical Associating Fluid Theory (sPC-SAFT) 2. Liquid – Liquid Equilibria and Prediction of Monomer Fraction in Hydrogen Bonding Systems«
■ Ioannic Tsivintzelis, Andreas Grenner, Ioannis G. Economou, and Georgios M. Kontogeorgis
(Submitted to Industrial and Engineering Chemistry Research)

SEP 0738
»Propane Hydrate Nucleation: Experimental Investigation and Correlation«
■ Lars Jensen, Kaj Thomsen, and Nicolas von Solms
(Submitted to Chemical Engineering Science)

SEP 0739
»Development, Modeling, Optimization and Scale-up of Chromatographic Purification of a Therapeutic Protein"
■ Jørgen M. Mollerup, Thomas Budde Hansen, Steffen Kidal, Lars Sejergaard, and Arne Staby
(Fluid Phase Equilibria, 261 (2007) 133-139)

SEP 0740
»The Thermodynamic Principles of Ligand Binding in Chromatography and Biology«
Jørgen M. Mollerup
(Journal of Biotechnology, 132 (2007) 187-195)

SEP 0741
»CO_2 Capture and Storage«
■ Amit Garg, Lars R. Appelquist, and Erling H. Stenby
(Risø Energy Report, 6 (2007) 25-29)

SEP 0742
»Study of Asphaltene Precipitation by Calorimetry«
■ Sylvain Verdier, Frédéric Plantier, David Bessières, Simon I. Andersen, Erling H. Stenby, and Hervé Carrier
(Energy & Fuels, 21 (2007) 3583-3587)

SEP 0743
»Development of a Migration model with an Implemented Agitation Parameter, especially for the use on GRINDSTED® SOFT-N-SAFE Migration from Polyvinyl Chloride«
■ Rasmus Lundsgaard, Georgios M. Kontogeorgis, Jørgen K. Kristiansen, and Torkil F. Jensen
(Submitted to Industrial & Engineering Chemistry Research)

SEP 0744
»Calculation of the Interfacial Tension of the Methane-Water System with the Linear Gradient Theory«
■ Kurt A. G. Schmidt, Georgios K. Folas, and Bjørn Kvamme
(Fluid Phase Equilibria, 261 (2007) 230-237)

SEP 0745
»A Computational Efficient and Robust Implementation of the Continuous-Discrete Extended Kalman Filter«
■ John Bagterp Jørgensen, Per Grove Thomsen, Henrik Madsen, and Morten Rode Kristensen
(Proceeding of the American Control Conference, New York City, USA, 11-13 July, 20078)

SEP 0746
»Equilibria in the Mixed Solvent System Glycol-NaOH-CO_2-Water Applied to Corrosion Modelling«
■ Philip Loldrup Fosbøl, Kaj Thomsen, and Erling H. Stenby
(ECCE6 proceedings, vol. 1 (2007) 137)

SEP 0747
»Classical and Recent Free-Volume Models for Polymer Solutions: A Comparative Evaluation«
■ Hamid Reza Radfarnia, Georgios M. Kontogeorgis, Cyrus Ghotbi, Vahid Taghikhani
(Fluid Phase Equilibria, 257 (2007) 63-69)

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