



DTU Chemical Engineering Annual Report 2012

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Publication date:
2012

Document Version
Publisher's PDF, also known as Version of record

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Citation (APA):
Dam-Johansen, K. (Ed.) (2012). DTU Chemical Engineering: Annual Report 2012. Technical University of Denmark, Department of Chemical and Biochemical Engineering.

DTU Library Technical Information Center of Denmark

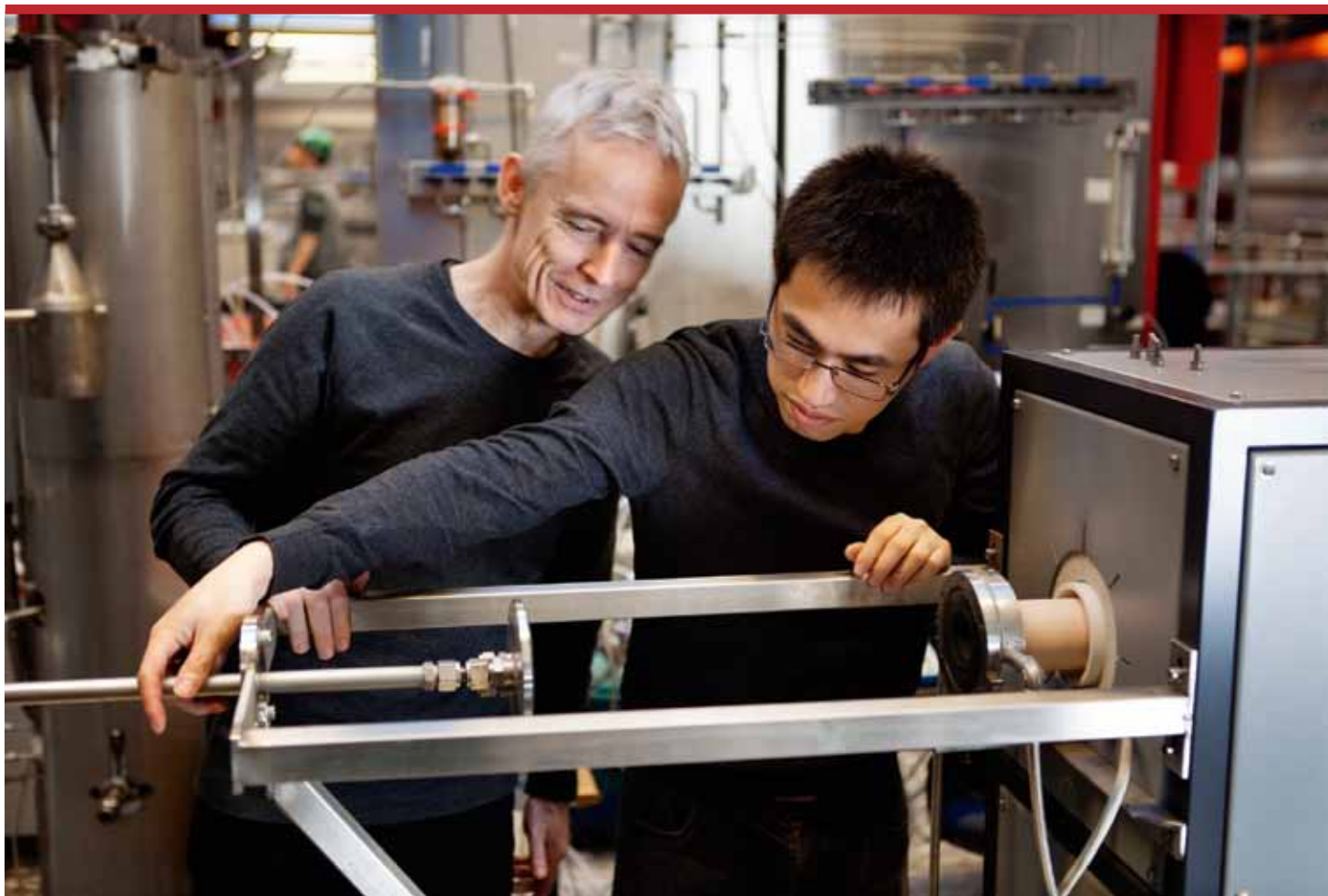
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Annual Report 2012



Annual Report 2012

March 2013

ISBN-13: 978-87-92481-90-0

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Design & Production

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Print

PE Offset A/S

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The background of the cover is a photograph of a modern building with a prominent red vertical section and a grey corrugated metal facade. Bare trees are visible in the foreground and background against a cloudy sky. The text is overlaid on a white rectangular area in the top right corner.

ANNUAL REVIEW

.....
Head of Department

HEAD OF DEPARTMENT

LEADING THE WAY IN A CHANGING WORLD



Kim Dam-Johansen
Professor, Head of Department

The world is changing. The present challenges differ from previous challenges – and we can be certain that next year will be different from this year. DTU Chemical Engineering has always been characterized as a dynamic organization ready to make timely changes in the way we work, the way we are organized and how we cooperate with our main stakeholders: brilliant undergraduate and graduate students, peers from academia all over the world and our demanding and loyal industrial partners who meet the pressure from their individual markets – to be still more effective –

to launch new and improved products and continuously to improve their competitiveness through higher efficiency, lower environmental footprints and by being attractive for the best graduates.

Constant Development to meet Future Challenges

Over the last decade we have grown and developed the department significantly. We have merged in the bachelor of engineering education from the previous Engineering Academy, we have initiated the transformation of the department to include and grow

the fields of Biochemical Engineering and Quantitative Product Design. We have step by step made the needed organizational changes and we have recruited brilliant Faculty members to lead the development. Today our activities within the new fields are fully integrated in both research and education. In other words we have moved the traditional Chemical Engineering activities linked to fossil fuels and energy systems into a modern Chemical and Biochemical Engineering department which in addition to the traditional and still very important fields also covers biotechnology,

pharma products and production, advanced soft materials, and formulated product design based on chemical engineering principles.

Significant Infusion of Skills and Competencies

Having succeeded in this development, 2012 was the year to make yet another important step by integration of activities from the previous Risø National Laboratory. On 1 January we welcomed around 80 new employees to our department, we reorganized our activities by merging in three groups in three existing research centers (PROCESS, BioEng and CHEC) at the department and by forming a new research center named ECO, with its main future focus on industrial ecology and sustainability in chemical and biochemical engineering. We expect this center to develop its activities over the coming years to become an integrated part of our core disciplines and to develop its field towards quantitative and well-defined methods to product and process sustainability evaluation based not only on

economic considerations but also on well-defined evaluation of environmental and climate footprints. On our teaching, this has already led to the development of three new courses on industrial ecology.

Reinforced International Cooperation

Another important development during 2012 has been our new focus on the cooperation with peers in Asia. We have established cooperation with Korean Advanced Institute of Science and Technology (KAIST) and we are presently working on a new education in Chemical and Biochemical Engineering with special focus on Biomass and Energy to be taught from September 2013 in Beijing in cooperation with especially Institute of Process Engineering (CAS) as part of the Sino-Danish Center for Research and Education.

A Valued Asset - Our Employees

The success of the department is dependent on our ability to attract the right people – employees and students – and to form a productive, deman-

ding and inspiring environment. This year I can welcome four new Faculty members: Research Specialist Hanne Østergaard, Professor MSA Kim Pilegaard, Associate professors Manuel Pinelo and Ulrich Krühne.

Together with colleagues at the department, I am convinced that our new faculty members will strengthen our capabilities for leading the way and continuously break new ground in the exciting world of chemical and biochemical engineering and thus prepare society and strengthen our industrial partners for the future.

I hope you will enjoy reading our 2012 Annual Report.



Kim Dam-Johansen
Professor, Head of Department





RESEARCH CENTRES & RESEARCH AREAS

AT CERE - Applied Thermodynamics - Center for Energy Resources Engineering

BIOENG - Center for BioProcess Engineering

CAPEC - Computer Aided Process-Product Engineering Center

CHEC RESEARCH CENTER

DPC - Danish Polymer Center

ECO - Ecosystems and Environmental Sustainability

PROCESS - Center for Process Engineering and Technology

AT CERE is a dynamic research group with an excellent track record and international reputation in the areas of applied thermodynamics, transport processes, and mathematical modeling. The center is committed to perform high quality experimental and theoretical research with international impact. There are extensive collaborations, first of all within CERE and DTU Chemical Engineering but also with universities and industries around the world. It shares the same industry consortium with CERE which in 2012 includes 29 companies, of which 22 are international.

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APPLIED THERMODYNAMICS - CENTER FOR ENERGY RESOURCES ENGINEERING AT CERE

THE CENTER IN BRIEF

AT CERE is the section of CERE at DTU Chemical Engineering. CERE was created in 2009, as a continuation and extension of the IVC-SEP center, and has activities across DTU. At DTU Chemical Engineering the main contributions are within the area of applied thermodynamics, mathematical modeling and transport in porous media. In close collaboration with industry, relevant authorities and international research organizations, the scientific results from AT CERE are implemented in various industrial products and processes.

AT CERE has five faculty members at DTU Chemical Engineering. These are Professor Georgios M. Kontogeorgis, Associate Professors Nicolas von Solms, Alexander Shapiro, Kaj Thomsen and Assistant Professor Philip Fosbøl. With the center are also associated a strong

technical and administrative staff as well as a software manager.

The main activities of AT CERE are in the areas of complex solutions (including polymers, electrolytes, biomolecules and associating chemicals), nonequilibrium thermodynamics (diffusion and thermo diffusion), and simulation of petroleum recovery processes. These skills are applied in several research projects of strategic importance such as CO₂ capture and storage, flow assurance and Enhanced Oil Recovery (EOR). CERE's Industrial Consortium is a valuable asset for research and education at DTU. Many companies provide financial support for research projects in addition to the membership. For instance, the Chemicals in Gas Processing project (CHIGP), which is extensively sponsored by industrial partners (cur-

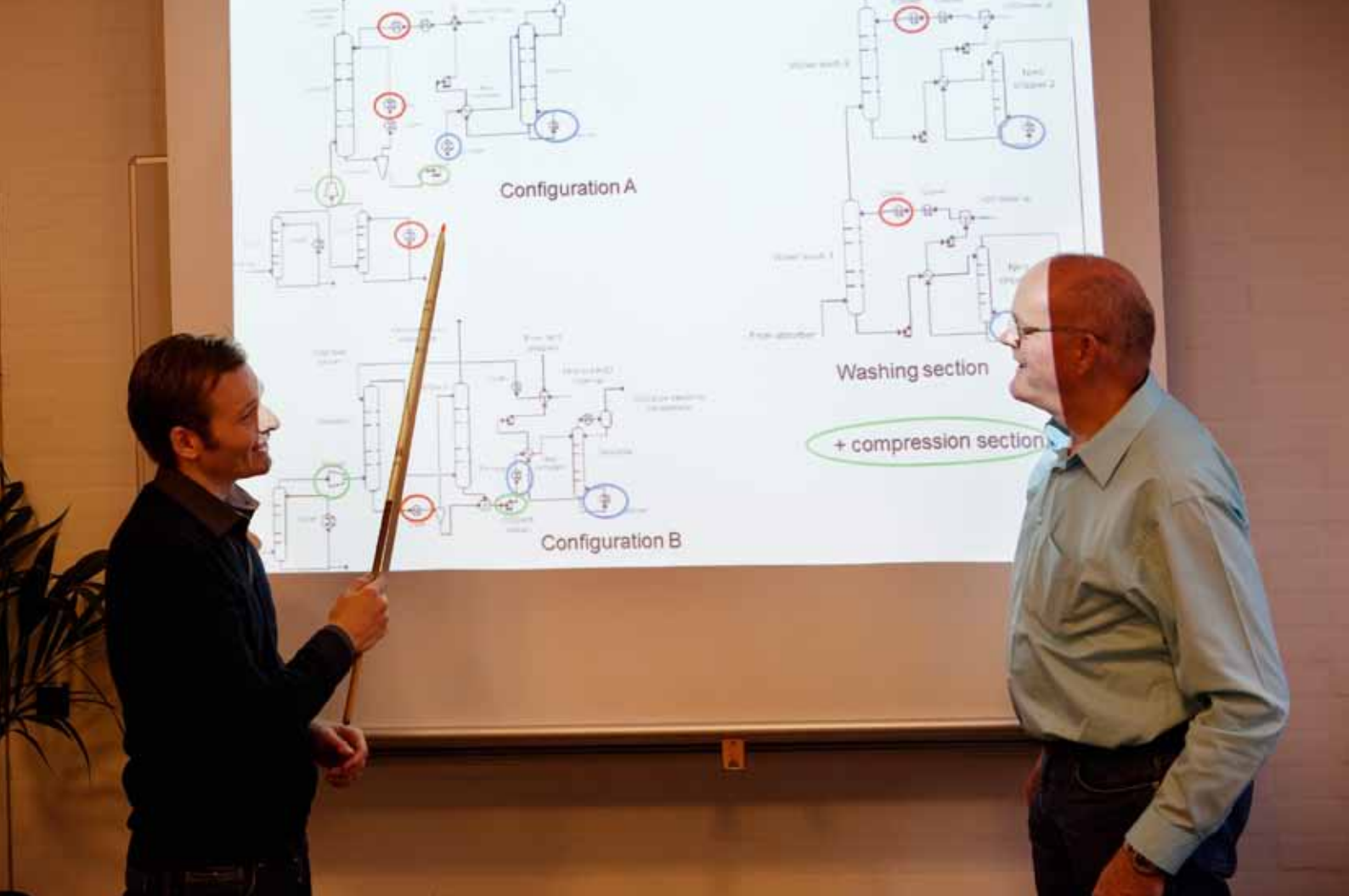
rently by Statoil, Gassco, DONG Energy, BP, and Petrobras).

RESEARCH AREAS AND EXAMPLES OF RESEARCH PROJECTS

The research activities at AT CERE are divided into the following three main activities:

- ➔ Thermodynamics and transport properties for petroleum and for complex fluids (associating fluids, polymers, electrolytes, surfactants, biomolecules)
- ➔ CO₂ capture and storage (CCS)
- ➔ Reservoir engineering and petroleum fluids - enhanced oil recovery (EOR)

Thermodynamics and mathematical modeling are the key disciplines, accompanied with modeling of transport properties, physical chemistry (especially colloids and interfaces), reaction



From left, Philip Fosbøl and Kaj Thomsen discussing the newly developed CERE extended UNIQUAC software package for Aspen Plus. Here it is applied to an electrolysytic simulation of CO₂ capture, using high pressure ammonia.

engineering and material science especially polymers.

Major deliverables include the development of databases (e.g. on electrolytes) and thermodynamic/unit operation software in diverse forms:

- ➔ SPECS for academic/educational use
- ➔ CAPE-OPEN / ASPEN user models – so that thermodynamic models can be used in commercial simulators

Another important activity are the PhD courses organized by the center's faculty on computational aspects and algorithms for thermodynamic calculations (Michael Michelsen), petroleum thermodynamics (Alexander Shapiro),

electrolytes (Kaj Thomsen) as well as statistical thermodynamics and molecular simulation (Nicolas von Solms and visiting professors).

Finally, the experimental facilities include measurements of thermodynamic and transport properties at low and high pressures as well as oil applications including a CT-Scanner. The experimental activities are led by Nicolas von Solms and supported by a competent team of 5 technicians.

A few examples of major (on-going) research projects are briefly outlined below.

THE CHIGP PROJECT

CHIGP (Chemicals in Gas Processing) is a joint industry project which started

in 2003. Currently the participating companies are Statoil, BP, DONG Energy, GASSCO, Petrobras (who joined in 2012), while previously (over 6 years each) TOTAL and Maersk Oil have also participated.

The target of the project is the development, support and dissemination of an advanced thermodynamic model, the CPA (Cubic-Plus-Association) equation of state. Emphasis is given on applications of interest to the petroleum and chemical companies.

The results are disseminated to the participating companies via CAPE-OPEN compliant modules and user-models for the ASPEN process simulator, all provided via a dedicated web-site.



Associate Professor Alexander Shapiro and his PhD students Amalia Halim (on the left) and Alsu Khusainova (in the middle) are discussing formation of emulsions and microemulsions due to interaction of oil with different solutions, containing various types of bacteria or enzymes.

POLYMERS

Polymer thermodynamics has traditionally been a focus area for the center, and various thermodynamic models have been developed, e.g. extensions of UNIFAC and cubic equations of state to polymer solutions and more recently the development of an equation of state (simplified PC-SAFT). The latter has been used in various applications for mixtures including polymers at low and high pressures. One application, in collaboration with NKT Flexibles, is the modeling of gas-polymer interactions (solubility and swelling) at high pressures. Another polymer-related project, in collaboration with Danisco, was the study of the migration of plasticizers from PVC, a study which combined

mathematical modeling and molecular simulation tools.

ELECTROLYTES

Electrolytes are present in numerous applications in the petroleum, energy and chemical companies. In many of these applications are present mixed solvents and salts over broad T/P conditions, e.g. for predicting scale deposition in oil and gas production. Major activities include the development of the extended UNIQUAC model, e.g. for applications related to CCS (see below) and recently also electrolyte equations of state (e.g. the extension of CPA mentioned above to electrolytes). Other applications where we will focus in the future include energy storage in

salt solutions and in phase change materials as well as recovery of phosphate from biomass.

GAS HYDRATES

Gas hydrates are typically considered a nuisance during oil & gas production and transport and should be avoided at any cost. For this reason, large amounts of thermodynamic inhibitors (methanol, glycols) are used. Even though advanced models (like CPA) can accurately model the thermodynamic properties of oil-gas-water-inhibitor systems which is important for the optimum use of these chemicals, still these are needed in big amounts and they are nasty chemicals! In collaboration with cryobiologists from Roskilde

University, we have looked at a very promising alternative, the use of the much more environmentally friendly anti-freeze proteins from arctic fish and insects as potential kinetic inhibitors of gas hydrates. The first results using these novel protein inhibitors are promising, and future challenges involve changing them in biochemical ways in order to become more effective and producing these proteins in larger amounts, e.g. via fermentation so that they can be tested in practical applications.

CARBON CAPTURE AND STORAGE (CCS)

CCS has been named by the US academy of engineering as one of the 14 grand challenges for engineers in the 21st century. In close collaboration with power companies (DONG Energy, Vattenfall) & other universities (via several EU-funded projects) and centers we have over the last 10 years carried out an extensive research program focusing on post-combustion capture of CO₂. In this direction, we have investigated the capabilities of various solvents (alkanolamines, chilled ammonia, ionic liquids, amino acids, carbonates, etc.) for capturing CO₂ from coal-fired power plants. Both experimental (lab and pilot-scale) and modeling studies have been carried out.

ENHANCED OIL RECOVERY RESEARCH

We participate in a series of innovative projects in the area of enhanced oil recovery (EOR). Studies of the salinity effect on EOR have been carried out in the framework

of the large ADORE project followed by the current SMARTWATER project. The last project is supported by the Danish Energy Agency and the petroleum companies: Maersk Oil and Gas, and DONG Energy. The project is run in collaboration with DTU Civil Engineering (Professor Ida Fabricius, coordinator of the project). Massive flooding experiments under varying salinity conditions are planned in the SMARTWATER program. These studies will be followed by the studies of the rock-oil-brine interactions and advanced thermodynamic and hydrodynamic modeling.

Another project, BIOREC, deals with the application of biological agents in petroleum industry. Three Ph.D. students and three post-doctoral researchers are currently working at AT CERE on the project, supported by the Danish National Advanced Technology Foundation, and the companies: Maersk Oil and Gas, DONG Energy, and Novozymes. The project is run in collaboration with the Danish Technological Institute and the Roskilde University. In the first work package of the project, an extensive experimental and modeling study is carried out.

A separate study, also related to oil recovery, was modeling of the filtration process: motion and deposition of the particles in a flow in a porous medium. The study has been carried out in the framework of project ParPor (Particles in Porous Media) supported by the Danish Council of Independent Research | Technology and Production Sciences (FTP).

In 2012 the CERE Consortium consisted of the following members:

.....
 Akzo Nobel (NL)

 BP (GB)

 Chevron (US)

 Conocophillips (US)

 DONG Energy A/S (DK)

 Eni (IT)

 ExxonMobil (US)

 GASSCO (NO)

 GDF-SUEZ (FR)

 Haldor Topsøe (DK)

 Hess (DK)

 Inchochem (GB)

 Linde (DE)

 Maersk Oil (DK)

 National Oilwell Varco (US)

 Petrobras (BR)

 RWE (DE)

 Saudi Aramco (SA)

 Schlumberger (US)

 Shell (NL)

 Sinopec (CN)

 Statoil (NO)

 SQM (CL)

 Total (FR)

 Vattenfall A/S (DK)

 Welltec (DK)

 Lloyd's Register ODS (DK)

 IFP (FR)

 OMV (AT)

Our mission is to provide new knowledge, new enzymes, new process strategies and products and to contribute to establish DTU as an internationally recognized University within the fields of enzyme technology and bioprocess engineering. At the same time our goal is to provide inspiring and pertinent teaching and student supervision in order to hatch top-qualified MSc and PhD candidates.

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CENTER FOR BIOPROCESS ENGINEERING - BIOENG

Center for BioProcess Engineering aims to provide new concepts for biorefining with a main focus on enzymatic processing of biomass. The research involves concept development for new processing routes, reaction strategies, and products design for improved raw materials utilization and production of platform compounds, biofuels, and food ingredients by use of biocatalysis. Biogas production from different substrates, including technology adaptation, is also a focus area in the Center.

Enzyme technology is the core research discipline in the Center. The research in the Center also involves *sustainability assessment* and *separation technology* research in the context of bioenergy and biorefinery processes. With the merger of the Bioenergy Group, Risø National

Laboratory of Renewable Energy in 2012, we are now 45 people in the Center for BioProcess Engineering, of which more than 20 are PhD students.

The research is structured into 5 core disciplinary topics

- ➔ **Enzyme Discovery and Food Ingredient Engineering**
Jørn Dalgaard Mikkelsen, Carsten Jers, Christian Nyffenegger + PhD students
- ➔ **Enzyme Technology**
Anne S. Meyer, Marcel Tutor Ale, Anis Arnous, Jesper Holck, Dayanand Kalyani, Anna K Sitarz + PhD students
- ➔ **Biofuel Production Technologies**
Zsófia Kádár, Pablo Kroff, Anders Thygesen + PhD students

- ➔ **Separation Technology**
Manuel Pinelo, Jianquan Luo + PhD students
- ➔ **Sustainability Assessment**
Hanne Østergård + PhD students

The research is supported by several key enabling technology platforms: i) Molecular biology and enzyme cloning, ii) Enzyme production, purification, and characterization, iii) chromatographical analyses platform (LC, GC), iv) bioethanol and biogas fermentation facility, v) biomass pre-treatment pilot. The research rests on a number of designated transdisciplinary topics: i) Enzyme kinetics, ii) Molecular enzyme analyses, iii) Advanced experimental design, iv) Emergy accounting and Meta system analysis.



Postdoc Marcel T. Ale is watching how lab technician Annette Eva Jensen loads samples for biomass monosaccharide composition analysis by HPAEC-PAD. This analysis is an important base for designing enzyme reactions on biomass.

Our mission is to provide new knowledge, new enzymes, new process strategies and products and to contribute to establish DTU as an internationally recognized University within the fields of enzyme technology and bioprocess engineering. At the same time our goal is to provide inspiring and pertinent teaching and student supervision in order to hatch top-qualified MSc and PhD candidates.

We collaborate closely with several different Danish and International companies and other Universities, with collaborators in Brazil, China, Ghana, Greenland, the US, and in various European countries.

ENZYMES

Enzymes are catalytic proteins and are defined as biological catalysts. By be-

ing catalysts, enzymes accelerate the rate of chemical reactions and work by lowering the activation energy of a given reaction. A unique trait of enzyme catalysis is the selectivity with respect to the reaction. This selectivity, or enzyme specificity, denotes that the enzyme catalyzes a specific reaction between specific chemical species to produce specific products. Enzymes are thus capable of catalyzing the conversion of certain compounds, i.e. enzyme substrates, present in a mixture, to specific products, and moreover able to work at mild reaction conditions. Enzymes can therefore be used in practical applications to catalyze processes that deliver energy, food, chemicals, materials, and pharmaceuticals in a sustainable way. The scientific foundation for developing all these applications is a profound un-

derstanding of enzymes and how they act as optimal catalysts.

ENZYME TECHNOLOGY: CONTENT AND PERSPECTIVES

Enzyme Technology is the research discipline that focuses on the design of new enzymes, enzyme catalyzed reactions, processes, and products. Enzyme Technology combines nature and technology, and our approach is to employ enzymes in bioprocessing. The design and development of new enzyme reactions and products obviously rely on detailed knowledge of natural enzymatic reactions and kinetics. In addition to enzyme discovery, the Enzyme Technology research in Center for BioProcess Engineering therefore involves enzyme protein engineering, microbial enzyme production, enzyme

action mechanisms, structure-function relations, reaction engineering and reactivity optimization, and kinetics.

One of the most immediate needs for society is to replace crude fossil oil as a core feedstock for many different products. At the same time it is crucially important to reduce CO₂ emissions, and enable the production of sufficient energy, materials, and food, for the world's increasing population. The perspectives are that Enzyme Technology can:

- » revolutionize the way we produce products
- » provide solutions that ensure sustainable raw material use
- » improve human health
- » address climate change problems

Classic enzyme applications include uses of enzymes in laundry detergents and in various food and beverage processes such as apple juice production and cheese manufacture, but more sophisticated enzyme applications have been developed more recently. A common denominator for the newer applications is the more knowledge-based, targeted use of a particular type of enzyme to catalyze a very specific molecular conversion. The newer applications thus exploit the unique specificities of enzymes as catalysts. The new direction of enzyme technology is to develop sustainable reactions in the sense that the enzymatic conversions can help 1. maximize the use of the raw materials (substrates) with 2. minimal use of energy and water, 3. minimal waste production, and replace current processes so that 4. the environmental impact and CO₂ emissions are reduced.

DEVELOPMENT OF HIGH-VALUE BIO-REFINERY PRODUCTS

Plant biomass, including agro-industrial residues resulting from e.g. sugar, starch, wine, juice, plant oil, beer, as well as first and second generation ethanol processing, is rich in carbohydrates having potential as building blocks to replace oil based products. Some of these carbohydrates also have biological activity as nutri-functional food ingredients. Plant biomass can therefore be feedstock for production of a range of new products, and concomitant production of higher value co-products can improve resource utilization and add economic value to most of the classical agro-industrial plant production processes. The biorefinery concept designates this production of different valuable products from the same crop or plant biomass stream. Development of targeted biomass conversion processes are a crucial prerequisite for unfolding the biorefinery potential of agro-industrial plant biomass. Because of their specificity, enzymes can assist in releasing, modifying, and converting specific biomass constituents, and provide new rational solutions for the separation of core components such as protein, carbohydrates, lignin, and selected high-value substances during biomass processing. Apart from the development of the designated enzymatic conversion processes, particular research challenges lie within the integration of separation technology including development of novel separation concepts for large scale processes, both upstream and downstream.

ENZYME TECHNOLOGY RESEARCH TRENDS

The new directions in enzyme technology are directed at developing new, more stable enzymes and more intense and efficient industrial enzyme processes:

- » Molecular evolution of enzymes for better robustness
- » Enzyme catalyzed synthesis reactions
- » Reactor design for optimizing enzyme catalysis
- » Process design to re-use enzymes

The progress in GMO technology has allowed the Center for BioProcess Engineering to develop a technology platform which provides a basis for enzyme engineering and production of gram amounts of specific, monocomponent enzymes. The aim is to produce of a range of enzymes for development and proof-of-concept demonstration of different enzymatic conversion technology concepts. The vision is that Enzyme Technology will play an important role in the development of sustainable processes in a fossil-free society.

INNOVATION POTENTIAL

In Europe in particular, the innovation of new reactions and products based on enzyme catalyzed conversions is an important research field as well as an important business area. Some of the Center for BioProcess Engineering's highlights in 2012 include new processes such as the enzyme assisted production of nutri-functional food ingredients¹, enzymatic reactions in non-conventional media², use of enzymes for designing food functionality³,



Associate Professor Manuel Pinelo working on ultrafiltration hollow fiber membrane used for continuous separation of bioactive compounds.

rapid analytical methods for predicting biomass conversion processes⁴, better understanding of enzyme kinetics of branched polysaccharide modification⁵, and improved foundations for membrane separation of bioproducts^{6,7}, and not least method evaluation for sustainability assessment on genuine systems (e.g. a farm)⁸. These achievements may pave the way for new science-based approaches to design of processes and products, including innovative biorefinery conversion processes and new actions for improving sustainability.

¹Expression and characterization of an endo-1,4- β -galactanase from *Emericella nidulans* in *Pichia pastoris* for enzymatic design of potentially prebiotic oligosaccharides from potato galactans (Michalak M., Thomassen L.V., Roytio H., Ouwehand A.C., Meyer A.S., Mikkelsen J.D.). *Enz Microb Technol* 50: 121-129, 2012.

²Thermodynamically based solvent design for enzymatic saccharide acylation with hydroxycinnamates in non-conventional media (Zeuner B., Kontogeorgis GM, Riisager A, Meyer A.S.). *New Biotechnol* 3: 255-270, 2012.

³Biocatalytic cross-linking of pectic polysaccharides for designed food functionality: structures, mechanisms, and reactions (Zaidel D.N.A., Meyer A.S.) *BioCat Agric Biotechnol* 1: 207-219, 2012.

⁴Rapid near Infrared spectroscopy for prediction of enzymatic hydrolysis of corn bran after various pretreatments (Baum A., Agger J., Meyer A.S., Egebo M., Mikkelsen J.D.) *New Biotechnol* 29, 293-301, 2012.

⁵Enzyme kinetics and identification of the rate-limiting step of enzymatic arabinoxylan degradation (Rasmussen L.E., Xu C., Sorensen J.F., Nielsen M.K., Meyer A.S.). *Biochem Eng J* 69: 8-16, 2012.

⁶Controlling the rejection of protein during membrane filtration by adding selected polyelectrolytes (Pinelo M, Ferrer C, Meyer A.S., Jonsson G). *Sep Pur* 85: 54-60, 2012.

⁷Statistical modelling of the interplay between solute shape and rejection in porous membranes (Vinther F., Pinelo M., Brøns M., Jonsson G., Meyer A.S.). *Sep Pur* 89:261-269, 2012.

⁸Assessing sustainability of a low-input single-farm vegetable box-scheme using emergy and LCA methodology (Markussen, MV, Kulak, M., Østergård, H, Nemecek, T). *Proceedings of SETAC 18th LCA Case Study Symposium: Sustainability Assessment in the 21st century*, 2012.

Center for BioProcess Engineering currently collaborates with the following industrial partners

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 Arla Foods Amba

DuPont|Danisco

DONG Energy A/S

Foss

KMC

Novozymes A/S

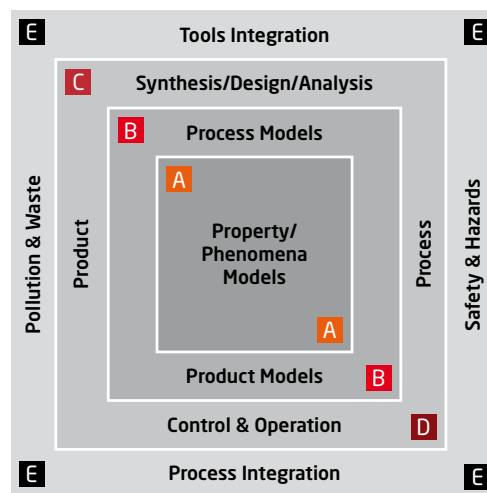
Briefly, the research objective of CAPEC is to develop computer-aided systems for efficient and reliable process simulation; for systematic synthesis, design and analysis of sustainable chemical products and their manufacturing processes; for robust control, operation and monitoring of processes from principally chemical, petrochemical, pharmaceutical and biochemical industries.

The computer-aided systems are to be developed based on fundamental and/or data-based modelling studies that incorporate correlation and estimation of thermo-physical and phase equilibrium properties as well as modelling the underlying principles / behaviour of the process-product. That is, by managing the complexity in a systematic and efficient manner.

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COMPUTER AIDED PROCESS-PRODUCT ENGINEERING CENTER - CAPEC

Research at CAPEC is organized in terms of six research programs (see Fig 1). At the inner most level (research programs A, B), the topics are related to fundamental research while at the outer most level (E), the topics are related to applied research. In the intermediate levels (C, D), systematic model-based algorithms, methods and tools are developed by employing the results from the inner levels for use in applied research in the outer level. Since all research programs need numerical tools and databases, research program F supplies this need to all levels.



The main theme of the research at CAPEC is to manage the complexity in the systematic analysis and solution of a wide range of product-process engineering problems from various industrial sectors.

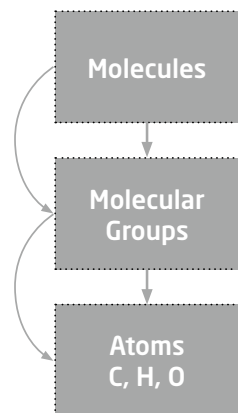
Figure 1: Organization of research in CAPEC in terms of research programs

Computer-Aided Molecular Design

From atoms to molecules

Lower Level of Aggregation

Next Lower Level of Aggregation



Computer-Aided Flowsheet Design

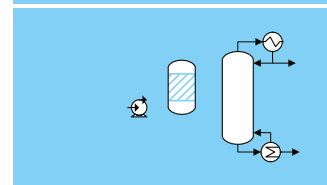
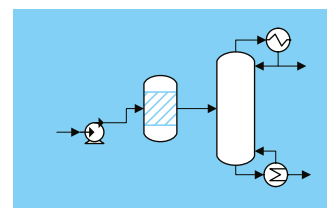
From phenomena to process

Flowsheet

Unit Operations

Tasks

Phenomena



Mixing Tasks

Reaction Tasks

Separation Tasks

Ideal Mixing

Reaction

2 Phase Mixing

Phase Contact

Phase Transition

Simultaneous product and process design at CAPEC

RESEARCH

The six research programs are briefly described below:

➔ **Research Program A – Property and Phenomena Modelling:** deals with theoretical studies of properties (pure component and mixture) of chemical systems and phenomena such as permeability through membranes, reaction kinetics and mass transfer through diffusion. A library of group contribution based models for a wide range of properties of organic chemicals is one of the highlights of program A.

➔ **Research Program B – Process-Product Modelling and Simulation:** deals with the development of models and model-based simulation systems for prediction of the behaviour and

performance of a wide range of chemical and biochemical processes (operating in batch, fed-batch and continuous modes) and a wide range of chemicals based products. A computer-aided modelling system for efficient model development and a collection of process-product models of various types, forms and scales are some of the highlights of program B.

➔ **Research Program C - Synthesis, Design & Analysis:** deals with the development and use of systematic algorithms, methods and tools for synthesis, design and analysis of chemical and biochemical processes and chemicals based products. Techniques such as computer aided molecular and/or mixture design (CAMD), and, process flowsheet design (CAFD) using the reverse

approach are some of the highlights of program C.

➔ **Research Program D - Process Control, Operation & Monitoring:** deals with the development and use of systematic algorithms, methods and tools for process control, operation and monitoring, including process analytical technologies. Techniques for tuning of controller parameters in model predictive control and methods for design of PAT systems are some of the highlights of program D.

➔ **Research Program E - Process and Tools Integration:** deals with on-line (process) and off-line (tools) integration as well as safety & hazards, sustainability analysis, and integration of process design-control, process-product

design and process-process. Integrated software such as ICAS, virtual process-product design lab, SustainPro and their associated methodologies are some of the highlights of program E.

→ **Research Program F - Database and Numerical methods:** since the CAPEC-PROCESS software needs to be self-sufficient in all respects for use by the industrial consortium companies, CAPEC also maintains a library of numerical methods and databases (properties of chemicals and solvents, reaction synthesis, membranes, and analysis equipments). The other research programs benefit from this in terms of data for modelling and improved simulation strategies.

Based on the above, the research objectives of CAPEC are summarized as:

Develop computer-aided systems for efficient and reliable process simulation; for systematic synthesis, design and analysis of sustainable chemical products and their manufacturing processes; for robust control, operation and monitoring of processes from principally chemical, petrochemical, pharmaceutical and biochemical industries. The computer-aided systems are to be developed based on fundamental and/or data-based modelling studies that incorporate correlation and estimation of thermo-physical and phase equilibrium properties as well as modelling the underlying principles / behaviour of the process-product. That is, by managing the complexity in a systematic and efficient manner.

CAPEC's research is focused - while the application horizon is wide (oil and gas, petrochemical, chemical and specialty chemical, pharmaceutical, food and bio

industrial sectors) the focus is on the use of a systems approach. CAPEC's strengths in terms of its research focus - pioneering work in certain research areas (such as modelling; methods for synthesis, design and analysis of processes as well as products; process and tools integration), industrial collaboration (dissemination of research results through the industrial consortium as well as collaboration with academia), and contacts (ability to influence developments within chemical engineering and CAPE/PSE). More specifically, CAPEC's contribution in the areas of thermodynamic property modelling for process-product design; computer-aided molecular-mixture design for consumer product development; targeted reverse approach for process intensification and integration; systematic computer-aided methods and tools for modelling, design, analysis and control are well known within the CAPE/PSE community.

PERSONNEL

CAPEC's permanent staff comprises Head of Center Professor Rafiqul Gani, Associate Professors Gürkan Sin and Jens Abildskov, Professor (Docent) Karsten Clement, Assistant Professor Jakob Kjøbsted Huusom and Secretary Eva Mikkelsen.

INDUSTRIAL CONSORTIUM

CAPEC has established an industrial consortium, where the PROCESS group is also involved. Through the industrial consortium, CAPEC-PROCESS co-workers have the unique opportunity to get quick and useful feedback on their developed models, methods and tools as well as insights to the current and future needs of the various industrial sectors represented by the consortium members.

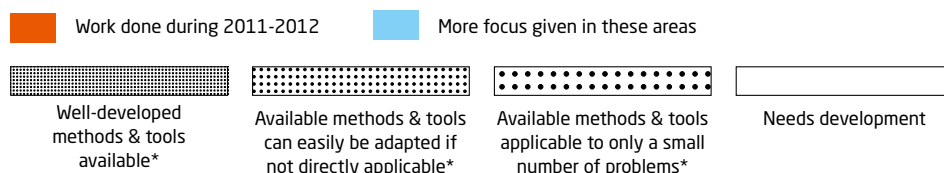
In 2012 CAPEC was supported by the following industrial consortium

Akzo Nobel (NL)
Alfa Laval A/S (DK)
AstraZeneca (SE)
BASF (DE)
Bayer Technology Services (DE)
ChemProcess Technologies (US)
Chemtura Netherlands B.V. (NL)
ConocoPhillips Company (US)
DSM (CH)
DuPont Nutrition and Biosciences Denmark (DK)
Firmenich (CH)
GlaxoSmithKline (US)
Huntsman Europe (NL)
Invensys Simsci-Esscor (US)
Janssen Pharmaceutica N.V. (BE)
Kongsberg Oil and Gas (NO)
Lonza AG (CH)
Mitsubishi (JP)
Navadan (DK)
Neste Jacobs Oy (FI)
Novozymes A/S (DK)
Optience Corporation (US)
Petrobras (BR)
Pfizer Inc (US)
Processium (FR)
ProSim (FR)
SCG Chemicals Co. Ltd. (TH)
Syngenta (GB)
Unilever Research (US)
VTT (FI)
Welcron Hantec Co. Ltd. (KR)

Table 1: Scope and significance of CAPEC research results shown in terms of industries where they can be applied

CAPEC Research Programs	Application of Research Results in terms of Industry					
	Petrochemical ¹	Chemical ²	Pharmaceutical	Agrochemical	Bio & Food	Aroma
Models & modelling tools						
Synthesis, design analysis & evaluation						
Control, operation & monitoring						
Process & tools Integration						
Databases & Numerical Methods						

¹: Includes also oil & gas industries; ²: includes also specialty chemicals



*Solving problems in process modelling, simulation, design, analysis and control

DISSEMINATION

The dissemination of the research results of CAPEC is carried out in terms of:

- » Computational Tools. Predictive models for reliable property estimation for a wide range of chemicals; generic mathematical models for process operation, product performance; computer-aided tools for product-process synthesis & design, etc., are used by leading industries and close to 50 universities from all over the world.
- » Technology: Developed systematic methodologies for process-product synthesis, design, analysis and

control (& operation), simulation strategies, solvent selection (& design), pollution prevention, sustainable process-product alternatives, etc., are routinely used to solve industrial problems and in education.

- » Application: Industrial case studies, tutorial case studies, technology transfer studies and consulting.

ACTIVITIES

The activities shown in Table 1.1 highlight the scope and significance of the research results available to the CAPEC-PROCESS industrial consortium members in terms of the industries where

the developed methods and tools are applicable.

Some of the challenges for the future are to use our methods and tools to find more sustainable alternative routes for the production of important chemical products in the petrochemical and chemical sectors using renewable and/or newly established resources; to help in the sustainable design/development of new and improved chemicals based products and the processes that manufacture them for the pharma, bio-food, agro and aroma industrial sectors; and, to incorporate in all problem solutions the issues related to energy, water, environment and green chemistry.

A vital part of our research is conducted in very close collaboration with industrial enterprises and international research organizations. The industrial relations cover close joint projects with a mutual exchange of staff and cooperation on experimental research ranging from microscale over pilot plants to full-scale industrial production plants. This approach ensures high relevance of our research and efficient exchange of technology, know-how and know-why.

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CHEC RESEARCH CENTER

CHEC is an acronym for Combustion and Harmful Emission Control. The Center was established in 1987 with the initial objective of employing chemical engineering principles in support of the efforts of the power industry to establish environmentally friendly processes – more specifically to build up basic knowledge to support the implementation of desulphurization processes and low-NO_x technologies for existing or new coal-based power plants.

Step-by-step CHEC has consolidated its industrial network and links to internationally recognized research organizations. CHEC has also expanded its research into new fields which are on par with its basic chemical engineering competence with special focus on Chemical Reaction Engineering. Today the main activities cover Industrial High Temperature Processes, Formation and Reduction of Harmful Emissions, Catalysis, Particle Technology and Quantitative Product Design and the recent merge with two groups from the previous Risø National Laboratory

has expanded the area of expertise to also cover Gasification processes and Advanced Diagnostic Tools for high temperature processes.

The primary vehicle for collection and storage of knowledge and knowledge transfer between different industrial applications is through experimentally verified mathematical models for gas phase reactions, gas-solid and catalytic reactions, condensed phase transformations etc. The models are typically developed and verified through experiments carried out at multiple scales, e.g. from small laboratory reactors to pilot scale and finally in full-scale in cooperation with industrial partners. The observations at full-scale often give important inspiration to further fundamental studies.

Within the new area of product design, CHEC has been able to achieve international recognition through a quantitative model-based approach. This field has a large potential both for chemical and biochemical products.

CATALYSIS - HEADED BY PROFESSOR ANKER DEGN JENSEN

The research focuses mainly on providing solutions to energy and environmentally related challenges and to develop green chemistry based processes. Present activities cover, among others, syngas conversion to alcohols, hydrodeoxygenation of bio-oil, steam reforming of bio-oil, DeNO_x for power plants and vehicles, catalytic soot combustion and more. The main objectives are:

- » To synthesize new catalytic materials by traditional wet chemical methods
- » Exploring flame spray pyrolysis (FSP) as a novel one-step preparation method for heterogeneous catalysts
- » To characterize the materials using spectroscopic and other techniques, and by theoretical means, such as density functional theory calculations (with partners), to understand and predict the properties of the materials
- » To test the activity, selectivity and deactivation of the materials under



Associate Professor Weigang Li operating a pilot-scale swirl burner to co-fire pet-coke and sewage sludge for the cement industry.

industrially relevant reaction conditions, and derive kinetic models including diffusion limitations applicable for reactor design

- » To model catalytic reactors and thereby obtain an improved understanding of the interplay between the process and the catalyst

Part of the activities is linked to the cross-department center, CASE, with cooperation with among others DTU Chemistry, DTU Center for Electron Nanoscopy and DTU Physics.

COMBUSTION AND EMISSION CONTROL - HEADED BY PROFESSOR PETER GLARBORG

The research focuses on the conversion of fossil and biomass-based fuels and the related formation and reduction of

pollutants. Working from small to very large scale with gaseous, liquid, and solid fuels, our main objectives are to develop predictive tools for combustion-related phenomena in power plants, waste incinerators, industrial processes, and engines. Specifically, we work in the following areas:

- » Characterization of pyrolysis, ignition, and char oxidation for alternative fuels (biomass, waste)
- » Characteristics of co-combustion of coal and alternative fuels in suspension
- » Development of chemical kinetic models for trace species formation and consumption in combustion – nitrogen, sulphur, halogens, alkali metals
- » In-situ processes for formation and control of harmful emissions

– NO_x, PAH, sub-micron particulates (incl. soot)

- » Experimental and modeling characterization of hydrocarbon and alcohol fuels oxidation at high pressure, and effect of ignition promoters
- » Oxy-fuel combustion

At present a large number of projects are carried out in close cooperation with power companies, boiler manufacturers and with the cement sector.

THERMAL GASIFICATION AND PYROLYSIS - HEADED BY SENIOR RESEARCHER ULRIK BIRK HENRIKSEN
Thermal gasification of coal and biomass may become important technologies both in combined heat and power production (CHP) and in the produc-

tion of liquid fuels and chemicals.

The work in CHEC cover activities ranging multiple scales and with a number of different technologies:

- » Low temperature gasification of low-grade biomass for co-firing in large scale power plants (PY-RONEER).
- » Up-grading of product gas from low temperature gasification by removing particles and converting the tars and use of the gas in Solid Oxide Fuel Cells
- » Optimization of small-scale biomass gasification systems for CHP, e.g. the DTU two-stage biomass gasification process
- » Utilization of nutrients and residual char in the ashes from biomass gasification and pyrolysis plants
- » Efficiency optimization of CHP gas engine operation on biomass gasification gas
- » Entrained flow gasification with minimal soot formation
- » Use of gasification gas for synthesis of liquid fuels and chemicals
- » Mobile biomass pyrolysis

PRETREATMENT OF BIOMASS - HEADED BY SENIOR RESEARCHER JESPER AHRENFELDT

Biomass as a raw material suffers from having a high specific volume and a soft texture making a grinding process difficult. In CHEC we work on different pretreatment methods such as torrefaction, pellets formation and pyrolysis to facilitate the future use of biomass in large-scale industrial processes. The present research covers:

- » Mechanical and chemical characterization of various biomasses towards grindability, durability, particle fluidization, humidification, composition, reactivity, thermal degradation, etc.
- » Development of a catalogue including an overview of characteristics of various raw and pre-treated biomasses
- » Field trials with storability of pelletized and torrefied materials
- » Combined torrefaction and milling of biomass
- » Up-scaling biomass pretreatment processes

INORGANIC CHEMISTRY - HEADED BY ASSOCIATE PROFESSOR FLEMMING FRANSEN

CHEC has for many years worked on inorganic metal species in high temperature processes and has established expertise in characterization of inorganic metal species in fossil and biomass-based fuels and on the interaction between the reaction environment and the transformations of inorganic species in different industrial processes. The research covers:

- » Release of ash-forming elements (mainly K, Na, Zn, Pb, S, and Cl) during devolatilization, pyrolysis, and subsequent char burnout in biomass combustion and waste incineration
- » Formation of aerosols from flame-volatilized ash-forming elements, like K, Na, S and Cl, and formation and entrainment of residual ash (i.e. bottom and fly ash) during char burnout in fixed-bed and suspension-fired systems

- » Transport of the different ash forming species gases, droplets and particles from the bulk gas to the heat transfer surfaces, and adhesion of these to the heat transfer surfaces
- » Build-up, sintering (consolidation), shedding, and heat transfer in deposits
- » A new lab-scale setup rotary kiln simulator (RKS) was designed and built to establish test equipment to simulate the industrial clinker burning process on a laboratory scale and to conduct clinker formation experiments in order to derive knowledge on gradual clinker property development, as a function of different process parameters
- » Sulfur release from cement raw materials during alternative fuel combustion including effects of temperature and gas atmosphere on the decomposition of sulfates in the raw materials has been investigated both experimentally and thermodynamically
- » Minerals process technology

DIAGNOSTICS - HEADED BY SENIOR RESEARCHER SØNNIK CLAUSEN

CHEC has from the very beginning combined fundamental studies in the laboratories with probe development to be able to diagnose what happens in larger scale industrial systems. By integration of the Optical Diagnostic Group from Risø this way of working today covers a number of different techniques used in on-going research:

- » Probes for deposition and corrosion (investigating the effect of flue gas composition, exposure time,

material choice, deposit chemistry etc.)

- » Probes for gas extraction, for measuring main gas components (CO₂, CO, O₂, NO_x, SO_x, alkali metals and aerosols)
- » Lambda probes for detecting redox conditions
- » Non-contact temperature, thermal radiation
- » Gas composition by spectroscopy
- » Optical flow measurements (laser, optics)
- » Imaging and visualization (UV, VIS and IR)
- » High-temperature gas cells (properties gases)
- » Optical sensors, instrumentation

reactor and unit operation designs and we have carried out fundamental and applied research on, for example, the following topics related to pharma production:

- » Design and operation of a mini filter reactor for continuous production of a selected pharmaceutical intermediate
- » Up-scaling and implementing a mini filter reactor in a pharmaceutical company
- » Design and development of continuous unit operations, e.g. crystallization, extraction etc.
- » Continuous reactors for Grignard reactions in general
- » Continuous reactors for slow organic chemical reactions

- and curing of thermoset coatings
- » Photoinitiated coating degradation of thermoset coatings
- » Drying of latex coatings
- » Anticorrosive coatings for corrosion prevention
- » Erosion resistant blade coatings for wind turbines

PRODUCTS AND PHARMA - HEADED BY ASSOCIATE PROFESSOR SØREN KIIL

CHEC's expertise in the traditional core disciplines Reaction Engineering and Transport Phenomena has been used in broadening the activities by the establishment of close cooperation to several companies working in the field of product design and batch production. The main aims are to incorporate more quantitative methods in the design and test of multi-component formulated products and to facilitate the transformation of batch-wise production to continuous or semi-continuous production. Projects in this field are often carried out in cooperation with faculty members at other centers. Converting a batch production into a continuous operation mode requires a detailed quantitative understanding of the chemical reactions involved. Our philosophy is to work on all relevant

In the field of product design and test, our main focus has been on heavy duty coatings as highly complex multicomponent products, which must fulfill many conflicting requirements. Our philosophy is to understand the main mechanisms behind coating behavior and we have carried out fundamental and applied research on, for example, the following topics:

- » Polishing and biocide leaching rates of antifouling coatings
- » Mapping of degradation routes for seawater-immersed anticorrosive coatings
- » Parameters influencing the performance of intumescent fire-protective coatings
- » Design of novel test equipment for antifouling and anticorrosive coatings
- » Simultaneous solvent evaporation

The CHEC Research Center primarily collaborates with the following industrial partners

Babcock & Wilcox Vølund A/S

B&W Energy A/S

Danish Gas Technology Center A/S

DONG Energy A/S

Energinet.dk

FLSmidth A/S

H. Lundbeck A/S

Haldor Topsøe A/S

Hempel A/S

Hwam A/S

MAN Diesel A/S

Novozymes A/S

Topsøe Fuel Cell A/S

Vattenfall AB

At the Danish Polymer Center we are devoted to the application of molecular design, synthesis and processing of polymers to create materials and products with unlimited ranges of properties and applications. We strive towards this goal in a balanced environment of education, research and industrial cooperation.

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DANISH POLYMER CENTER

- DPC

Denmark does not have any significant production of bulk polymers. Hence one might be surprised to find a center devoted to education and research in polymer science and engineering at DTU. However Denmark does have a large and diverse industrial sector devoted to the transformation of bulk polymers to a range of polymeric products. Typically these products are so-called high-end market products that are dependent upon highly trained researchers and engineers for their development and production. In order to maintain and develop this important activity in Denmark it is therefore of the utmost importance, that there is a supply of highly trained candidates in polymer science and engineering. In fact the DPC-DTU is the only center in Denmark with Masters level courses that specialize in the entire range of disciplines from polymer chemistry and physics to polymer engineering.

Simply put: The mission of the DPC-DTU is to train candidates for the Danish polymer industry.

RESEARCH AT DPC-DTU

The research is interdisciplinary ranging from chemical synthesis, chemical and physical characterization of polymers and soft materials to fluid mechanics of complex fluids. Current research areas include the synthesis of polymers with controlled molar mass, branching structure and functional groups, design of soft polymeric networks and rheology of polymer melts, solutions and emulsions. In 2012 the center had 5 faculty members and 1 research manager:

- ➔ **Ole Hassager:** Transport phenomena, polymer physics, and polymer rheology.
- ➔ **Søren Hvilsted:** Polymer chemistry and synthesis.
- ➔ **Peter Szabo:** Computational Fluid Mechanics, rheology and complex fluids.
- ➔ **Anne Ladegaard Skov:** Polymer gels and networks
- ➔ **Anders Daugaard:** Polymer materials and functionalized polymer surfaces.

- ➔ **Katja Jankova:** Methods for controlled synthesis of functional polymers.

Laboratories and Instrumentation:

Located in newly refurbished laboratories, the center has a very broad range of instrumentation for polymer synthesis and characterization:

NMR spectroscopy, Size Exclusion Chromatography, Infrared Spectroscopy, Cryo Ultramicrotome, Thermogravimetric Analysis, Differential Scanning Calorimetry, Contact Angle Measurements, Mechanical Spectroscopy, Shear Rheometry, Extensional Rheometry and Dielectric Spectroscopy.

EVENTS IN 2012:

On 30 November the DPC-DTU hosted the **8th Annual Polymer Day**, a one-day conference welcoming a wide audience including industry representatives from corporate Danish heavyweights such as Novo Nordisk and Coloplast. The event gives students the opportunity to present their work in an open forum. Fifteen presentations were held in Eng-



Kim Chi Szabo is loading the autosampler of the TGA Instrument with 7 polymer membranes in order to investigate the amount of surface grafted conducting polymer, and its influence on their thermal stability.

lish by DPC students with names and accents reflecting many different regions of the world.

Postdoc **Nicolas J. Alvarez** received the best poster award at the AIChE Annual Meeting in Pittsburg, Pennsylvania, USA. In its announcement, the American Institute of Chemical Engineers (AIChE) wrote: “Nicolas J. Alvarez was awarded the postdoctoral best poster award from the Fluid Mechanics division of the American Institute of Chemical Engineers in October of 2012 for his work on extensional creep measurements of low density polyethylene (LDPE). This work settles a long-standing controversy among rheologists by confirming the existence of steady extensional viscosity in LDPE melts.

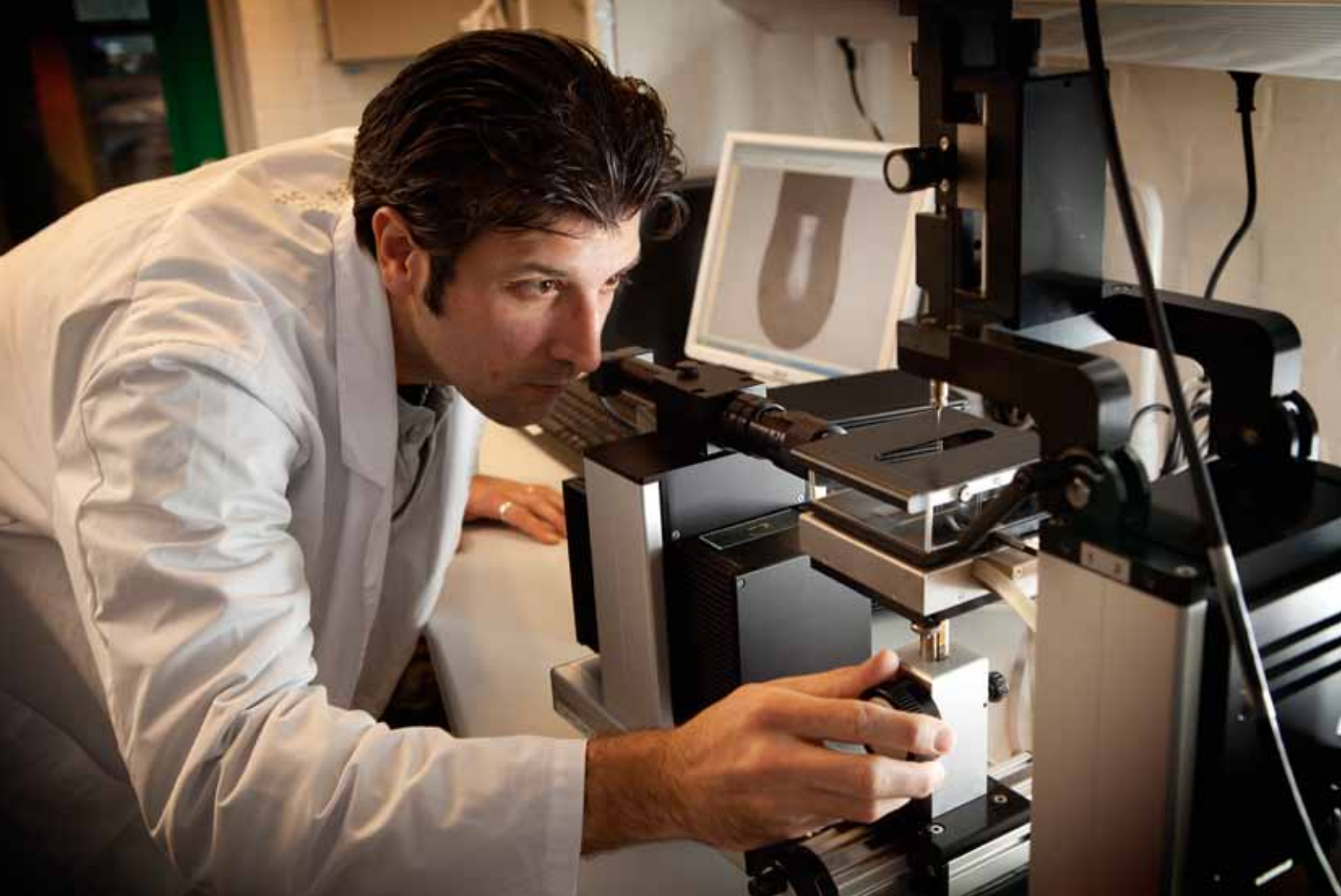
These results derive from the first and unique adaptation of a filament stretching rheometer to operate in constant stress mode devised by Nicolas and co-workers.”

Ph.D. student **Frederikke Bahrt** received the best poster award at the Nordic Polymer Days 2012. This year the 49th Nordic Polymer Days (NPD) took place in Denmark. NPD is arranged each year and hosted at turns in Sweden, Finland and Denmark. 126 polymer professionals from all the Nordic countries had signed up for the event. Frederikke Bahrt of DTU Chemical Engineering, Danish Polymer Center received the award for her poster presentation on “New Cross-Linkers for PDMS Networks”. Following up on

this, Frederikke won the iPad at the 6th European Silicon Days Conference in Lyon, France in September. Frederikke’s presentation was on Development of new PDMS based materials for dielectric electroactive polymers (DEAPs) as actuators and generators.

FUTURE FOR POLYMER MATERIALS

Today more than 99% of all polymer materials are based on fossil resources such as oil and gas. This fact frequently leads to the question of what future materials will look like after depletion of the fossil resources. The answer is, however, that most likely the importance of polymer materials will continue to grow completely unaffected of the price of crude oil for several reasons. First of all, it is only about 5% of the crude oil



Nicolas Alvarez operating the pendant drop/contact angle apparatus, which allows for the accurate measurement of interfacial and surface tension of liquids and polymer melts. The image in the background is that of pendant drop of POM suspended in a silicone oil.

that is used for polymer production. Since the Danish polymer industry produces high market products, the price of the raw material contributes a minor part of the price of the product. More importantly, however, alternative sources of raw material may become commercially competitive. Bio-based raw materials may become interesting in the near future. In the longer run, shale gas and oil from hydraulic fracking may

contribute to the raw material supply. Whatever the source of the monomers, the fundamental principles of polymer chemistry and physics remains the same. Hence the Danish industry will need candidates in polymer science and engineering for years to come. Thus the DPC-DTU will be needed in years to come.

COLLABORATION

The wide range of research areas related to polymeric materials gives great opportunity for project collaboration with the polymer processing industry. Close relations to industrial companies are maintained by an industrial consortium as well as through specific research projects or consultancy.

The Danish Polymer Center primarily collaborates with the following industrial partner

Alfa Laval Nakskov A/S (DK)

Coloplast A/S (DK)

Dana Lim A/S (DK)

Dyrup A/S (DK)

Grundfos Management A/S (DK)

Hempel A/S (DK)

Novo Nordisk A/S (DK)

Tetra Pak Packaging Solutions AB (SE)

MINERAL OIL CONSUMPTION IN WESTERN EUROPE <http://www.plasticseurope.org>

Energy and heating	45%
Transportation	42%
Polymers	5%
Other	8%



The ECO center at DTU Chemical Engineering conducts research to understand and demonstrate environmental impacts of technologies and industrial processes in chemical and biochemical engineering in order to assess and analyse the environmental sustainability

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ECOSYSTEMS AND ENVIRONMENTAL SUSTAINABILITY

- ECO

SUSTAINABILITY AND CHEMICAL ENGINEERING

The ECO center at DTU Chemical Engineering conducts research to understand and demonstrate environmental impacts of technologies and industrial processes in chemical and biochemical engineering in order to assess and analyse the environmental sustainability.

Sustainability is a global challenge – recently emphasized by UN High-level Panel on Global Sustainability in their report “Resilient People, Resilient Planet: A Future Worth Choosing”. The report provides 56 recommendations to advance visions for a sustainable planet, a just society and a growing economy. Future development will therefore require engineers with skills to ensure “sustainable engineering”. Engineers in chemical and biochemical engineering have to design and develop technologies

and industrial solutions that minimize resource use and prevent environmental impacts such as climate change. Detrimental effects on ecosystems and plant production must be avoided, the contribution of biological systems to exchange carbon dioxide and other greenhouse gasses must be taken into account and the growing demand and consumption of biomass for energy and biorefinery must simultaneously ensure the long-term fertility of our soils. Developing and conducting environmentally sustainable technologies is not “simple”. It requires careful consideration of all steps in the complex chain of processes from generating resources and feedstocks, their conversion to products and the handling of waste streams. The sustainability of technologies must be evaluated and assessed by Life Cycle Assessment (LCA) or other assessment tools and concepts. Finally

such evaluations and assessments need to be validated against “real-world” measurements of the impacts on the environment. ECO conducts research and teaches future engineers how to test and prove the sustainability of technologies in chemical and biochemical engineering through measurements and modelling of impacts and benchmarking against relevant and realistic sustainability metrics. This research will form the basis for teaching sustainable engineering.

INDUSTRIAL ECOLOGY

ECO’s research and teaching are embedded in the concept of “industrial ecology” (IE) - the study of material and energy flows through industrial systems, where analogies from ecosystem concepts of optimized energy and resource use and closed cycle thinking are applied to benchmark industrial processes

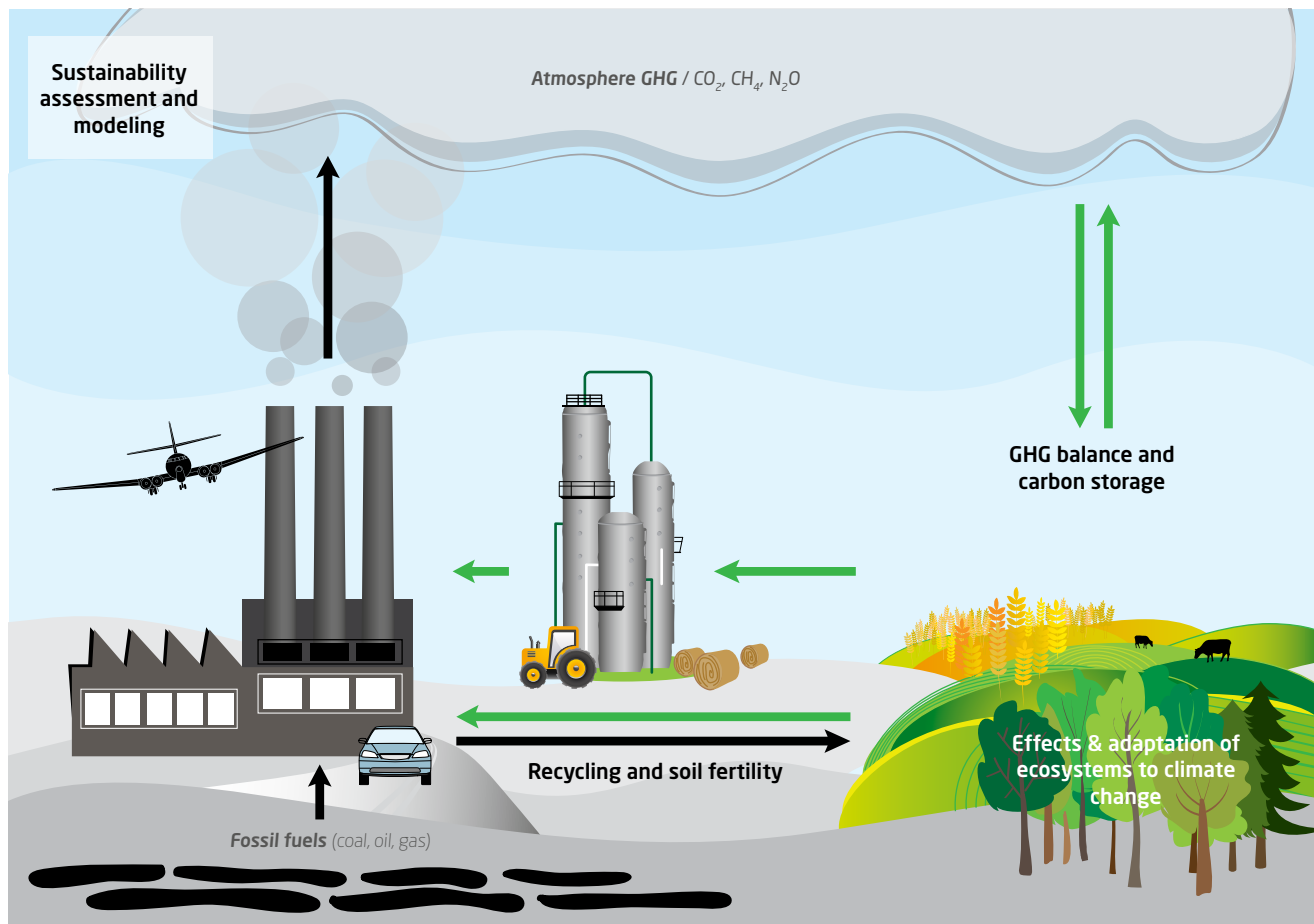


Figure 1: Key research areas of ECO aiming at assessing the sustainability of fossil fuel based energy production and industrial processes as well as new alternative processes based on biomass. The sustainability assessment involves laboratory and field based measurements and experiments testing the greenhouse gas feedbacks to the atmosphere, carbon storage in terrestrial ecosystems, climate change effects on terrestrial ecosystems and “closed cycle” concepts with recycling and reuse of waste streams to increase carbon storage and soil fertility.

and systems. Industrial ecology considers the technological world and the environment as one system linked via impacts and resources. Biomaterials are likely to become main organic resources for future chemical engineering, but the sustainability of bioresources is increasingly questioned. Direct and indirect impacts via climate change, eutrophication and over-exploitation compromise sustainability and narrow down the future boundaries of industrial activity and human welfare. Designing sustainable industries requires careful planning and considerations of the global system as a whole.

ECO approaches this new scientific teaching and research area through joining its ecosystem perspective with the chemical engineering competence of the Department. This integration is unique among chemical engineering departments but requires considerable efforts of communication and mutual understanding and will, therefore, take years for its robust development.

ECOSYSTEM STUDIES ACROSS SCALES – FROM GENE TO ECOSYSTEM

ECO has expertise and facilities to conduct realistic experiments and

measurements on plants and ecosystems to evaluate environmental impacts and sustainability of energy and chemical engineering technologies.

Environmental impacts can become manifested at a range of scales from genetic and molecular changes over ecotoxicity and loss of individual species to large scale changes in ecosystem structure and functioning. Therefore, studies of environmental impacts need to consider this span in scales. ECO is among the leading research groups in the world conducting long-term field GHG balance observations and designing and conducting realistic experiments in full



ECO employs and develops new advanced measurement techniques to study ecosystem processes. Here, ECO has developed a new advanced automatic chamber to measure uptake and release of CO₂ from plants and soil in order to evaluate the net effect of environmental and climatic changes on the ecosystems ability to take up and store carbon. These measurements are a fundamental requirement when long term sustainability in relation to climate change is to be evaluated.

scale ecosystems in order to investigate impacts of single and multiple factors. ECO's research is based on and employs state of the art research facilities including

- » laboratories to study chemical, biochemical and biological processes
- » field-scale facilities in natural ecosystems to conduct monitoring and realistic experiments at the microbial, plant and ecosystem scale
- » field trials for biomass and agricultural plant and growth tests

These facilities provide opportunities to experiment and measure crucial parameters to address environmental impacts on ecosystem processes and functioning such as soil structure and functioning, nutrient cycling, plant growth and adaptation, toxicity of waste streams from industry, climate feedback from ecosystems etc.

RESEARCH AREAS

➔ Effects and adaptation of ecosystems to climate change (e.g. impacts of elevated CO₂ on ecosystems and genetic adaptation of

plants) - research conducted by Claus Beier, Teis Mikkelsen, Rikke Bagger Jørgensen

Environmental impacts may lead to changes in plant performance and plant production with ramifications for both biodiversity as well as food and energy production. The sensitivity of plants and plant communities and the ability of these to adapt to new conditions are crucial for future adaptation strategies as well as technological development. ECO carries out effects studies providing insight on these changes at all scales from genes to the ecosystem.

➔ Carbon storage and greenhouse gas balances for ecosystems (e.g. carbon uptake in forests and non-CO₂ GHG emissions from energy crops) - research conducted by Kim Pilegaard, Andreas Ibrom, Per Ambus, Klaus Steenberg-Larsen and Mette Sustmann Carter

The ability of ecosystems to mitigate climate change through uptake or release of greenhouse gasses (i.e. their GHG balance) depends largely on internal carbon and nitrogen cycling, which are extremely sensitive to the physical and chemical environment and to management. At ECO we conduct research to increase our understanding on the feedback processes and how biomass production systems and utilization of bioresidues should be managed in order to help mitigate global warming. Typical timescales of the involved processes vary from short (30 minutes) to long (decades and more). Thus, field studies at ECO last from a few months to several decades.

➔ Soil fertility and recycling from biomass-based industries (e.g. biochar, ash recycling, anaerobic digestates, C, N, P cycling) - research conducted by Henrik Hauggaard-Nielsen and Iver Jakobsen

Terrestrial ecosystems deliver goods and services to society such as food

and fibres for energy and materials. The long-term sustainability of these services depends to a large extent on soil fertility. Soil fertility in plant and biomass production can be obtained through recycling of waste streams and by-products from the processes and technologies using the biomass and/or through optimizing plant processes with respect to nutrient use. ECO focuses on the development of possibilities to combine the plant production and production of bioenergy from biomass resources with conservation of soil fertility and soil carbon sequestration by means of redistributing the residual products to agricultural soils and/or optimizing the uptake and use of nutrients by plants.

➔ Ecosystem modelling and sustainability assessment (e.g. Life Cycle Assessment) - research conducted by Claus Beier, Andreas Ibrom and Rikke Bagger Jørgensen

The complex processes of ecosystems can be predicted within known uncertainty boundaries with process-based models. Models are core elements of all kinds of applications that consider ecosystem responses from individual impacts studies, to future global climate projections. Measurements and model outputs on ecosystem responses to environmental changes provide the basis for sustainability assessments.

Collaboration and Public Sector Consultancy

We collaborate with universities, EU, policymakers, public companies and private industry. We hereby apply concepts and results derived from our research to practical problems. In this way we also ensure dissemination of our research. Based on our key competences within climate change and sustainability we provide advice to public authorities and carry out joint research projects. Recent examples include risks associated with genetically modified organisms (GMO) and optimal utilization of biomass for bioenergy.

Ecosystems and Environmental Sustainability currently collaborates with the following industrial partners

-
- DLF Trifolium (DK)
- VEGA Solar Panels (DK)
- DONG Energy (DK)
- HedeDanmark (DK)
- Bregentved Estate (DK)
- AgroTech (DK)
- Videncenter for Landbrug (DK)
- Carlsberg (DK)
- Nordic Seed (DK)
- Sejet Plant Breeding (DK)
- GramiNor (NO)
- Sw Seed/Lantmännen (SE)
- Boreal
-

The vision of the Center for Process Engineering and Technology is to provide the necessary support to enable the next generation of processes to be implemented in industry. In this way, the new developments in biotechnology, catalysis and separation science alongside process engineering can be translated into industrial practice. New processes with reduced waste, high efficiency, and based on all the principles of sustainability can be developed which will help develop the European industrial sector in the production of chemicals, bio-based materials and chemicals, as well as pharmaceuticals.

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CENTER FOR PROCESS ENGINEERING AND TECHNOLOGY - PROCESS

BACKGROUND

The Center for Process Engineering and Technology (PROCESS) was created in January 2010. The primary objective of the work in the Center is to provide the necessary research and support for industry to develop and implement the next-generation of chemical, pharmaceutical and fuel production processes. The next generation of processes, which will be implemented in industry between 5 and 15 years from today, will be clean with an excellent environmental footprint and using the latest technology for reaction and the subsequent product recovery steps, as well as advanced process control built around mechanistically-based process models. In PROCESS we are working with many of the major companies to match their expectations in terms of what these processes will make and the technology and support infrastructure

required. Many processes of the future will involve nature's catalysts (biocatalysts) and for this reason fermentation and biocatalysis are important subjects. The biocatalysis group is led by John Woodley (campus Lyngby) and the microalgae group by Klaus Breddam (campus Risø). Supporting the development of these new technologies are two other groups. The dynamic modeling group is led by Krist Germaey (campus Lyngby) and is focused on dynamic models primarily built on a mechanistic basis to gain an understanding of unit operations and processes. Computational fluid dynamics and population balance models are also important elements of this work. The final group is focused on miniaturized processes and is led by Ulrich Krühne. Miniaturized processes find application both in process development as well as production, dependent upon the industry sector

and type of process. The sub-groups are supported by an excellent team of postdocs, PhD students as well as many masters and bachelor students.

BIOCATALYSIS

A key technology for the next generation of processes will be biocatalysis (the use of one or more enzymes or cells containing one or more enzymes for the production of chemicals, pharmaceuticals and fuels). Biocatalytic processes offer the advantage of un-paralleled selectivity under mild reaction conditions. Nevertheless when using biocatalysis on non-natural reactants, rates are often low and conditions frequently sub-optimal. This has led to the development of improved enzymes via recombinant DNA technology. At PROCESS we work with both academic and industrial partners who supply recombinant enzymes and cells for us to



Multiphase reaction media (using dyed organic or aqueous phases for visual studies) is a feature of many of the new biocatalytic systems.

use and test in entirely new processes. In order to complement this we focus on the novel engineering concepts which are also required for the final effective implementation of such processes (especially where the reaction thermodynamics is unfavorable). The work is mostly experimental, based both in the laboratory (in miniaturized and scaled-down equipment) as well as the pilot plant. In addition some research is focused on methodology to implement and develop biocatalytic processes in the most effective way including economic and environmental evaluations, which is essential to ensure the sustainability of such new processes. The sub-group cur-

rently works on several enzymes such as transaminases (for the synthesis of (chiral) amines), lipases (for the synthesis of biodiesel), oxidases and oxygenases (for the selective introduction of oxygen into molecules). Process concepts include multi-enzymatic processes, substrate feeding, in-situ product removal and multi-phase processes. The work is funded by several EU projects, including BIOINTENSE which we launched in 2012.

MICROALGAE

Some microalgae contain large amounts of triglycerides, in particular when they are subjected to stress. As The mission

of the microalgae sub-group within PROCESS is to reduce the costs of microalgae based oil production. This will be achieved by development of more efficient algae characterized by higher growth rates and increased capacity to produce oil in a controlled manner. As an example, we have isolated temperature sensitive cell-cycle mutants of *Chlamydomonas reinhardtii* with the aim to identify mutants that over-produce neutral lipids when challenged by higher temperatures. Crucial indicators for the selection of these mutants at the restrictive temperature are a block in cell division but not for growth. As a result, the cells increase in size as a visi-



Anne Olsen and Claes Gjermansen studying microalgae that can produce plant oil.

ble phenotype. Among the temperature sensitive mutants 9 out of 41 mutants in *Chlamydomonas reinhardtii* and 11 out of 53 in *Chlorella vulgaris* accumulated neutral lipids at the restrictive temperature under nutrient replete conditions. In a collaborative effort with Chinese Academy of Science, Qingdao Institute of Bioenergy and Bioprocess Technology we are also establishing a synthetic biology platform in the lipid producing algae *Nannochloropsis* allowing genome engineering to introduce new genetic traits.

DYNAMIC MODELING

The third sub-group in PROCESS is concerned with dynamic modeling. Mechanistic models – mathematical models developed based on mass, heat and momentum balances – as well as process simulation and advanced model

analysis will play an increasingly important role for fermentation process development. The mechanistic model can be supplemented by a modeling toolbox including uncertainty and sensitivity analysis to assess the statistical quality or reliability of the model predictions. An important feature of mechanistic models is that they allow extrapolation of the data to understand the effects under untested conditions. Therefore, when available, those models can be used within process design and optimization to exploit opportunities for process improvement which have not been tested experimentally. The required size of the reactor will, for example, depend strongly on the achievable conversion rates – rates that can be predicted with the mechanistic model. However, taking industrial fermentation as an example, the majority of the new products

typically do not involve design of a new plant, but rather fitting the new reaction or strain and/or separation scheme into existing equipment. In this case, availability of a reliable process model, for example developed on the basis of pilot-scale experimentation, enables *in silico* investigations of the process performance under different operation conditions before moving to full-scale. In this way, introducing new products/strains is more efficient, since it can rely on the mechanistic model to evaluate the necessary trade-offs that will be needed in order to allow establishment of an efficient new production process within the constraints of the existing equipment.

Models become increasingly complex, for example as the result of including additional details in a model. Computational fluid dynamics (CFD) is used to

model spatial distribution of reactants and hydrodynamics. CFD model applications are expected to become more common to support the optimal exploitation of existing production capacity in the fermentation industry. CFD can be taken a step further, and can be combined with models describing cellular metabolism.

MINIATURIZED PROCESSES

The rapid development of microfluidic technology has the past years contributed to the development of a number of novel technologies used in diagnostics, molecular biology, medicine and process engineering. In chemical and biochemical engineering the production of fine chemicals or chemicals with low production volumes has thus far been in focus of this enabling technology. Miniaturized systems have in general the advantage that:

- » Excellent material transport can be achieved as a result of short diffusion lengths and active flow for instance controlled by pumps
- » Superior heat transfer is ensured as well due to short energy transport distances and small volumes which have to be heated or cooled
- » Minute amounts of precious materials can be investigated
- » Biological reactions e.g. with immobilized cells or enzymes can be controlled also with respect to physiological conditions (shear stress)
- » High chemical and biochemical conversion rates can be achieved due to the fact that the reactions are often transport limited (diffusion)

- » Due to the small feature sizes of the channels nearly always a laminar flow pattern occurs. This means mixing will take place by diffusion only.
- » Due to the laminar flow character the fluid dynamic behaviour can be precisely predicted by use of numerical methods (computational fluid dynamic (CFD) methods have solely to solve the Navier Stokes equations).

Those advantages are expected to contribute significantly to the experimental investigation of complicated reaction schemes. Development of microfluidic experimental platforms will contribute to process screening and characterization. It is expected that the systems will help to cheaply and reliably access

- » kinetic data,
- » material characteristics (diffusion, solubility),
- » optimal operation modes (continuous, batch, fed batch, segmented flow, plug flow),
- » stability /activity of enzymes,
- » solvent screening, immobilization modes (packed bed, membrane, wall-coated).

Coupling the experimental screening methods with dynamic modeling and use of mechanistic models it will be possible to reduce the amount of tedious and time consuming experiments and to accelerate in this way the classical way of development of new technology and processes. This will result in a reduced time to market for future product

development in the field of chemical and biochemical engineering.

COLLABORATION

A key feature of PROCESS is collaboration with the very best scientists and engineers. Within KT we have collaborations at all levels and with each of the other centers. Likewise we have many academic collaborators via EC funded projects around Europe. Primary collaborators include The University of Manchester (UK), University College London (UK), TU Graz (Austria), LTH (Sweden), TU Dortmund (Germany), Slovak Technical University (Slovakia), Copenhagen University (Denmark).

The nature of the research work means that collaborations are not only required with academic scientists but also industrial engineers and scientists working in both the research and also developments part of companies. Both large companies as well as small and medium sized entities (SMEs) are essential to such collaborations. Major industrial collaborators include Novozymes (Denmark), Novo Nordisk (Denmark), BASF (Germany), c-LEcta (Germany), CLEA technologies (The Netherlands), DSM (The Netherlands), Evonik Industries (Germany), Astra Zeneca (Sweden).

In addition PROCESS is part of the CAPEC-PROCESS industrial consortium, which provides an excellent forum for discussion of process systems engineering (PSE) based tools and methods applicable to the next generation of production processes.

HIGHLIGHTS 2012



b-value experimen
August 2012 - Octo





1) Associate Professor Anne Ladegaard Skov with one of the DEAP materials, photo: Stefan Mogensen. 2) Professor Anne S. Meyer on national news, photo: TV2 3) Eirini Karakatsani receives Best Poster award at 3rd International Gas Processing Symposium in Qatar.

HIGHLIGHTS 2012

JANUARY

JANUARY 1

Parts of Risø National Laboratory formally become part of DTU Chemical Engineering

Approximately 80 new employees become part of DTU Chemical Engineering. The employees come from Risø Biosystems and Risø Plasma Physics and Technology Programme. An intense integration process is initiated to welcome the new employees and to maximise the synergy effects obtained.

JANUARY 26-27

Nordic Process Control Workshop NPCW17

The 2012 NPCW was hosted at DTU and jointly organized by DTU Chemical Engineering and DTU Informatics. The workshop brought together 100 participants, with 30 coming from the industry.

JANUARY 30

Inauguration Lecture by professor Georgios Kontogeorgis

Professor Kontogeorgis gives a lecture on his field of excellence, Applied Thermodynamics. The inauguration lecture is attended by more than 80 guests, including colleagues from DTU, the industry and other institutions.

FEBRUARY

FEBRUARY 7-8 ①

DEAP Symposium

The DEAP project's 50 member strong research team meets at DTU for a first symposium – sharing latest news and results and giving a general status of the project. At the core of the project is research carried out by Associate Professor Anne Ladegaard Skov and her team at the Danish Polymer Center (DPC) at DTU Chemical Engineering. The project is supported by the Danish National Advanced Technology Foundation.

FEBRUARY 23 ②

Professor Anne S. Meyer features on national television

Professor Anne S. Meyer features on national television, TV2, on the subject of bioethanol. Professor Meyer appears on television on the background that Novozymes is presenting a new enzyme that may render the production of bioethanol both less expensive and easier to accomplish.

MARCH

MARCH 5-7 ③

Eirini Karakatsani awarded Best Poster at 3rd International Gas Processing Symposium

Eirini Karakatsani, postdoc in AT CERE, was awarded Best Poster at the 3rd International Gas Processing Symposium for her poster "Towards the modeling of natural gas systems containing water and selected chemicals".



4) Associate Professor Ulrich Krühne with Dr. Peter Pind (right) of Novozymes, photo: Stefan Mogensen. 5) PhD student Frederikke Bahr of DPC receives the Best Poster Award at the Nordic Polymer Days. 6) Professor Rafiqul Gani of CAPEC welcoming industry partners, photo: Deenesh Babi.

MARCH 12-13

AT CERE joins EU project OCTAVIUS

AT CERE joins the OCTAVIUS (Optimization of CO₂ Capture Technology Allowing Verification and Implementation at Utility Scale) project funded under the 7th EU framework program for research (FP7).

APRIL

Nominations to the Management Committee for COST Action TD1107

Senior Researcher Henrik Hauggaard-Nielsen is nominated as member to the Management Committee for COST Action TD1107 – Biochar as an option for sustainable resource management. Senior Researcher, Jesper Ahrenfeldt is nominated as Substitute to the Management Committee.

APRIL 26 ④

Nordics BioProcess Improvement Seminar 2

DTU Chemical Engineering and DTU Systems Biology hosted a seminar on bioprocess innovation across different scales. The emphasis was on best practices, novel solutions, process intensification and single use technologies. Approximately 40 people from the industry and universities took part in the seminar.

APRIL 26

ECO welcomes two visiting Professors from Adelaide, Australia

Professors Sally Smith and Andrew Smith, The University of Adelaide worked for two months with ECO to investigate effects of future climate conditions on phosphorus uptake by plants.

MAY

MAY 10

Debate Day about Bioenergy, Food and Ethics in a Globalized World

The Danish Council of Ethics and CONCITO held a debate day at the Danish Parliament. Senior Researcher Rikke Bagger Jørgensen, who sits on the ethics council, took part in the day which was opened by the Danish minister for Climate, Energy and Building, Martin Lidegaard.

MAY 14

ECO Workshop on sustainable use of phosphorus reserves

The workshop was organized by Iver Jakobsen and co-workers with 16 participants from seven countries, including Danish plant breeders. Focus was on the capacity of symbiotic mycorrhizal fungi to increase root phosphorus uptake.

MAY 29-31 ⑤

Nordic Polymer Days 2012

The Danish Polymer Center (DPC) of DTU Chemical Engineering was well represented at this year's Nordic Polymer Days. PhD student Frederikke Bahr of DPC was awarded Best Poster Award for her presentation on New Cross-Linkers for PDMS Networks. NPD is arranged each year and hosted at turns in Sweden, Finland and Denmark. 126 polymer professionals from all the Nordic countries had signed up for the event.



7) Agnete Gørløv and Andreas Hofer win 2nd prize in Grøn Dyst, photo: DTU. 8) Head of Department Kim Dam-Johansen and Per Olesen (right), Vice President of Novozymes.

HIGHLIGHTS 2012

JUNE

JUNE 12-14 ⑥

CAPEC-PROCESS Industrial Consortium Annual Meeting 2012

On 12-14 June 2012, CAPEC and PROCESS held their second joint Annual Meeting with close to 90 participants from their industrial partners and academia. The subjects of the presentations encompassed modelling, physical property data, process-product design, process analysis control and monitoring, and software improvements.

JUNE 13-15

CERE Discussion Meeting

CERE Discussion Meeting 2012 took place on 13-15 June with 94 participants, including 22 of the center's consortia and academia partners. The topics covered at this year's meeting were: Complex Fluids, CO₂ Capture and Storage, Geoscience, Reservoir Engineering and Petroleum Fluids.

JUNE 22 ⑦

Students at DTU Chemical Engineering win 2nd and 3rd prizes at GRØN DYST

Two bachelor students, Agnete Gørløv and Andreas Hofer, win the 2nd prize in the bachelor project category at GRØN DYST. Agnete and Andreas' bachelor project is focused on 2nd generation bio-fuels; supervisor is Professor Anker Degn Jensen. Master student Jan Erik Nielsen wins the 3rd prize for his master thesis on diabatic distillation; supervisor is Associate Professor Jens Abildskov.

JUNE 29 ⑧

Novozymes Donates DKK 10 Million to Professorship in Industrial Fermentation

Novozymes and DTU initiate a partnership which significantly boosts research in industrial fermentation technology. The collaboration means that Novozymes establishes a new professorship at the department. In connection with the donation, Per Olesen, Vice President of Novozymes and responsible for developing production processes, production technologies and products at Novozymes, states, "We have a long-standing tradition for a sound and fruitful partnership with DTU Chemical Engineering, and this professorship is a natural part of our collaboration."

JULY

JULY 15-19

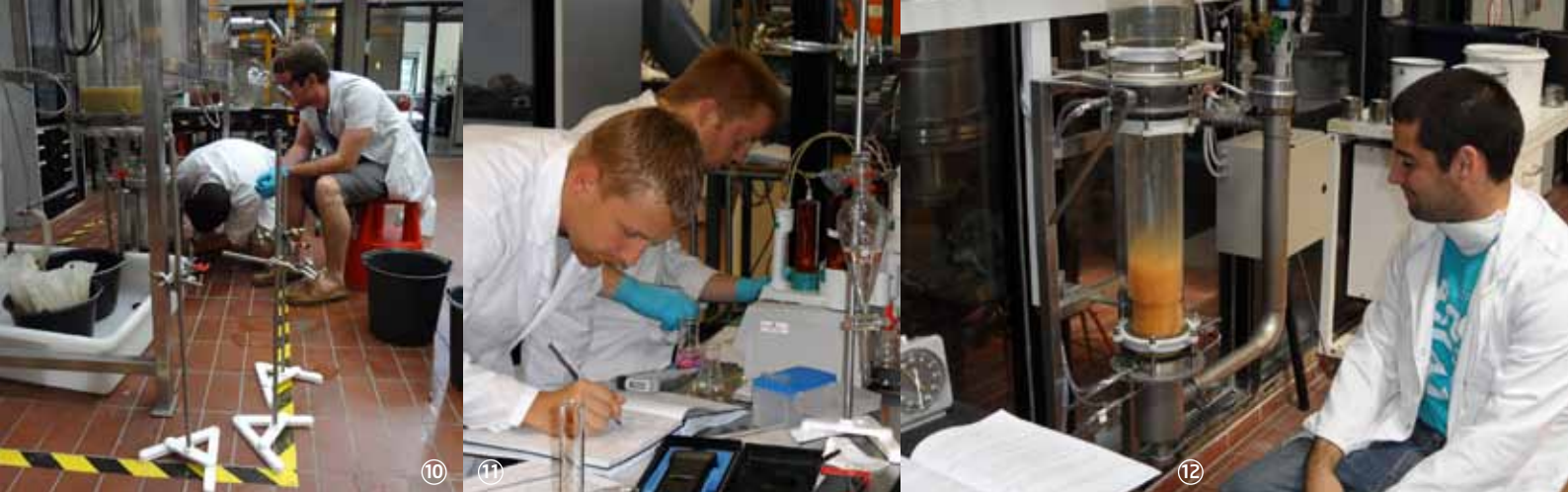
CAPEC & PROCESS Researchers Attend PSE2012 in Singapore

A nine-strong team from CAPEC and PROCESS attended the conference in Singapore to advertise that our department will be hosting the next international symposium, PSE2015, as a joint event with ESCAPE25 in 2015.

JULY 2-29 ⑨ - ⑫

Summer University at DTU Chemical Engineering a Continued Success

The Summer University again attracted many students from especially the USA. In total 53 students took part in the summer course which is focused on unit operations at the department's unique pilot plant.



9-12) Summer University at DTU Chemical Engineering, photo 9,11,12: Lars Kjørboe, photo 10: Stefan Mogensen.

AUGUST

AUGUST 1 ⑬

Sønnik Clausen celebrates 25 years at Risø and DTU

Senior Researcher Sønnik Clausen celebrated his 25th anniversary at Risø and DTU. Sønnik Clausen works with advanced instrumentation at the CHEC Research Center.

AUGUST 13-24

Advanced Course on Thermodynamic Models

As part of the department's continuing education offers, the Advanced Course on Thermodynamic Models: Fundamentals & Computational Aspects was conducted. The principal teacher at the course was Docent Michael L. Michelsen. Participants were researchers and PhD students from USA, Germany, Brazil, Italy, India, Norway, Czech Republic and Denmark.

AUGUST 23-24 ⑭

KAIST-DTU Collaboration Workshop on Biorefining

DTU Chemical Engineering welcomed its cooperation partners from the Department of Chemical and Biomolecular Engineering at KAIST to further discuss possible areas of collaboration – in a workshop on definition of a common Biorefinery programme. Many promising areas of collaboration were identified, on both research, students exchange and teaching.

AUGUST 27-31

Course on Coatings Science and Engineer

Associate Professor Søren Kiil conducts a five-day course for eight participants from the coatings industry. The course is part of the department's offers on continuing education for external parties.

SEPTEMBER

SEPTEMBER 1

Four new members of faculty

Former Head of Biosystems Division at Risø, Kim Pilegaard, is appointed Professor in Chemical Engineering with special assignments (MSA). Dr. Manuel Pinelo and Dr. Ulrich Krühne are employed as Associate Professors. Research Specialist Hanne Østergård also joins our faculty.

SEPTEMBER 19

Workshop on Biocatalytic Process Design

The PROCESS research center organizes a meeting for the European Network BIOTRAINS in Copenhagen. The meeting was followed by a two-day workshop on Biocatalytic Process Design at DTU, which included a visit to Novozymes A/S facilities.

SEPTEMBER 21

Krist V. Gernaey receives research grant from the Novo Nordisk Foundation

Associate Professor Krist V. Gernaey receives a grant from the Novo Nordisk Foundation to pursue a research project on exploring biochemical process performance limits through topology optimization.

SEPTEMBER 26-27

International ecosystem modelling workshop

The ECO center organized an international ecosystem modelling workshop in Copenhagen for the INCREASE EU project with representatives from six different European climate change



13) Sønnik Clausen celebrates 25 years at Risø and DTU, photo: Henriette Christensen. 14) KAIST-DTU Collaboration Workshop, photo: Christian Ove Carlsson

HIGHLIGHTS 2012

experiments as well as invited modeling experts. The aim was to obtain improved model predictions of the effects of climate change on ecosystem processes through standardized model application across multiple climate change experiments.

OCTOBER

OCTOBER 8-13 ⑮

DTU Chemical Engineering Conducts Autumn School in Beijing

Scientists from CHEC, DTU Chemical Engineering were in Beijing in October to conduct an Autumn School at Institute of Process Engineering, Chinese Academy of Science. The delegation from DTU Chemical Engineering conducted the course on thermal and catalytic conversion of biomass and waste, including the subjects of combustion, pyrolysis, gasification, ash chemistry and advanced instrumentation. A subsequent workshop comprised presentations from 25 scientists – evenly distributed between the two countries.

Kim Dam-Johansen in Beijing to prepare new joint MSc programme

Professor Kim Dam-Johansen visits Beijing to prepare for a coming MSc programme in Chemical and Biochemical Engineering (Biomass & Energy) as part of the Sino-Danish Center for Education and Research.

OCTOBER 23-24

Students visit BASF in Germany

25 bachelor and master students of DTU Chemical Engineering and Assistant Professor Jakob Kjøbsted Huusom went to BASF, the world's leading chemical company. The visit both gave an insight into the classical chemical areas of BASF based on oil and natural gas – and an insight into BASF's biotechnology research. The latter served as a good illustration of real-life process design, and lab to large-scale issues.

OCTOBER 25

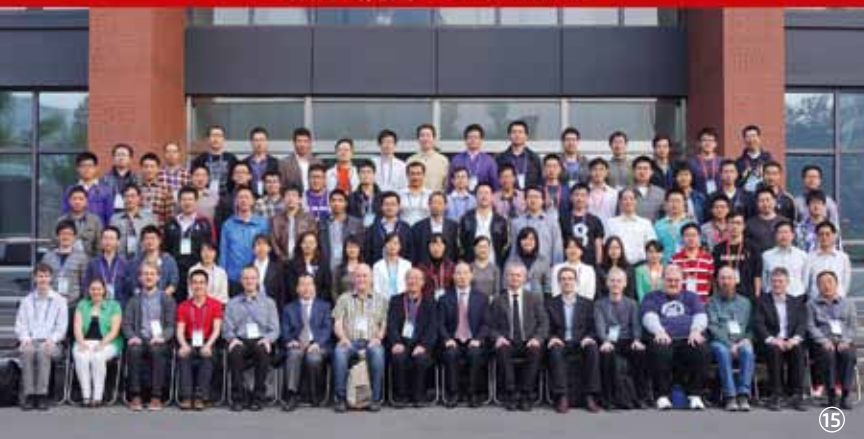
First workshop of the BIOPRO consortium

Associate Professor Krist V. Gernaey and Professor John M. Woodley participate in the BIOPRO consortium, a collaboration project between DTU Chemical Engineering, KU-Life, DONG Energy, Novo Nordisk, Novozymes and CP Kelco aiming at establishing bio-based production processes with increased efficiency.

OCTOBER 26 ⑯

Technician Jens Henry Poulsen celebrates 25 years in the workshop

Jens Henry Poulsen has worked for 25 years in the workshop at DTU Chemical Engineering. Jens and his colleagues deliver an excellent service to the department signified by high skills and commitment.



15) Autumn School in Beijing, photo: IPE-CAS. 16) Jens Henry Poulsen celebrates 25 years in the workshop, photo: Christian Ove Carlsson. 17) Postdoc Nicolas Alvarez next to the FSR, photo: José Marin. 18) Frederikke Bahrt (left) wins Best PhD presentation at the Christmas Meeting, photo: Nina Thomsen.

OCTOBER 29 ⑰

Postdoc Nicolas Alvarez Receives Best Paper Award at AIChE Annual Meeting

Postdoc Nicolas J. Alvarez of the Danish Polymer Centre (DPC) at DTU Chemical Engineering received the award at the AIChE Annual Meeting in Pittsburgh, Pennsylvania, USA.

NOVEMBER

NOVEMBER 8

Launch of new EU project BIOINTENSE

Professor John M Woodley, Associate Professor Ulrich Krühne and postdoc Pär Tufvesson launch the new EU project BIO-INTENSE which they coordinate together with Associate Professor Krist V Gernaey. The kick-off meeting was held in Brussels with all partners.

NOVEMBER 30

DPC 8th Annual Polymer Day

The Danish Polymer Center (DPC) holds its 8th Annual Polymer Day with 50 participants from industry and academia. Keynote speaker was Professor Julian Evans, Professor of Materials at the Department of Chemistry, University College London.

NOVEMBER 30

Professor Anne Meyer celebrates 25 years at DTU

Professor Anne Meyer celebrates her 25 years at DTU. Anne Meyer wrote her PhD at DTU, Department of Biotechnology

(later DTU BioCentrum) where she worked until 2006 when she was employed as Professor and Head of the Center for BioProcess Engineering at DTU Chemical Engineering.

DECEMBER

DECEMBER 14 ⑱

Annual Christmas Meeting at the department

The annual Christmas meeting brought together all staff of the department for a day of professional knowledge transfer and mingling. The programme included 12 presentations from PhD students – arranged as a competition with short 3-minute presentations among which colleagues could vote for the best three. Frederikke Bahrt won 1st place with her presentation “New Cross-linkers for PDMS Elastomers as Artificial Muscles”. The day also included presentations from the 7 research centers. Head of Department Kim Dam-Johansen gave a status on the department and an outlook into 2013.

DECEMBER 17

Professor Anker Degn Jensen in new catalyst project with Haldor Topsøe

On 17 December the Danish National Advanced Technology Foundation (Højteknologifonden) announced that they support a joint DTU Chemical Engineering and Haldor Topsøe A/S project on the development of new catalysts for heavy diesel-powered vehicles. The foundation grants DKK 9.5 million for the 4-year project bringing the total budget of the project to DKK 19 million.



A blurred background image showing several people in a meeting or collaborative work environment. One person in the foreground is wearing a blue and white striped shirt, and another person in the background is wearing a dark sweater. The overall scene is out of focus, emphasizing the text overlay.

PRODUCTIVITY

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Staff 2012

Productivity

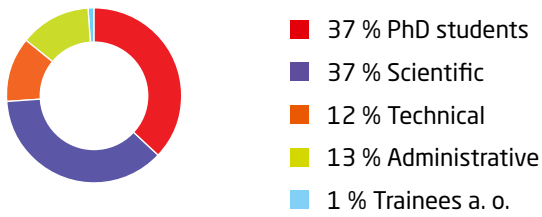
Publications

Education

STAFF 2012

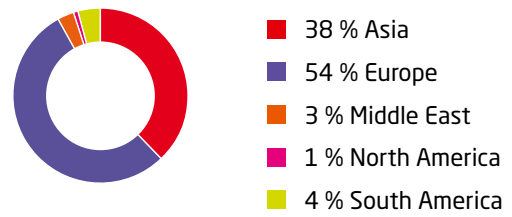
TYPE OF STAFF

(Total 268 persons)



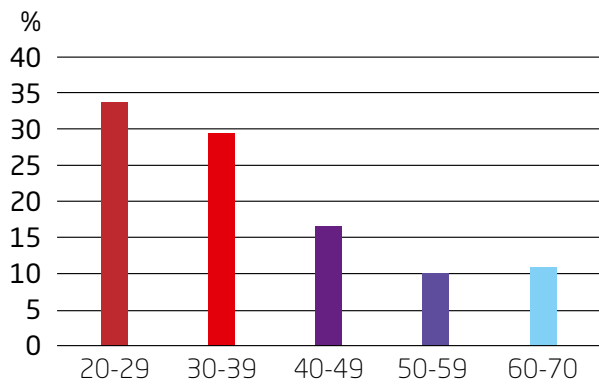
FOREIGN SCIENTIFIC STAFF

(Total 101 persons)



STAFF DISTRIBUTED BY AGE

(Total 268 persons)



PRODUCTIVITY

TEACHING & EDUCATION 2012

STUDENTS, EDUCATIONAL RESOURCES AND IMPACT

Students (STÅ*)	192
Completed BSc projects	20
Completed MSc projects	59

* One STÅ is the equivalent of one student studying full time in a year

RESEARCH & INNOVATION 2012

Scientific articles with referee in ISI-indexed journals (WoS)	170
Scientific articles with referee (non-WoS)	17
Contributions to refereed conference proceedings (and book series)	26
Monographs	1
Contributions to books	9
PhD Theses	29
Scientific publications and conference contributions with no peer-review	138
Contribution indicated as popular	9
Scientific reports	4

PUBLICATIONS

Scientific articles with referee in ISI-indexed journals (WoS)

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Arvaniti, E.; Bjerre, A.B.; Schmidt, J.E. (2012): **Wet oxidation pretreatment of rape straw for ethanol production.** *Biomass & Bioenergy*, 39, 94-105.

Avlund, A.S.; Kontogeorgis, G.; Michelsen, M.L. (2012): **Application of simplified PC-SAFT to glycol ethers.** *Industrial & Engineering Chemistry Research*, 51(1), 547-555.

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MASTER'S AND BACHELOR COURSES

The department participates in a 3½ year education for the Bachelor of Engineering, a 3 year education for Bachelor of Science and a 2 year education for the Master of Engineering. Below, course numbers and names are shown for 2012, with the number of students attending shown in brackets. Courses for Bachelor of Engineering are marked with (B). The other courses are Master courses or common courses.

SPRING SEMESTER

28012 Chemical and Biochemical Process Engineering (28) (B)
 28016 Mathematical models for chemical and biochemical systems (20) (B)
 28017 Chemical and Biochemical Process Engineering (18) (B)
 28020 Introduction to Chemical and Biochemical Engineering (62)
 28022 Unit Operations of Chemical Engineering and Biotechnology (23) (B)
 28121 Chemical Unit Operations Laboratory (16)
 28122 Chemical Unit Operations Laboratory – Summer University for Europeen (3)
 28157 Process Design (22) (B)
 28160 Mathematical models for chemical systems (34)
 28212 Polymer Chemistry (20)
 28214 Polymer Synthesis and Characterization (6)
 28221 Chemical Engineering Thermodynamics (20)
 28231 Laboratory in Chemical and Biochemical Engineering (24)
 28322 Chemical Engineering Thermodynamics (16) (B)
 28342 Chemical Reaction Engineering (29) (B)
 28345 Chemical Reaction Engineering (23)
 28350 Process Design: Principles and Methods (44)
 28352 Chemical Process Control (29) (B)
 28415 Oil and Gas Production (36)
 28423 Phase Equilibria for Separation Processes (19)
 28434 Membrane Technology (36)
 28443 Industrial Reaction Engineering (31)
 28451 Optimizing Plantwide Control (13)
 28850 Quality by Design (QbD): Integration of product and process development (24)
 28852 Risk Assessment in Chemical Industry (29)
 28855 Good Manufacturing Practice (55)
 28864 Introduction to Matlab Programming (26)
 28885 Technology and Economy of Oil and Gas Production (26) (B)

Courses given in cooperation with other departments:

26316 Analysis and Chromatography (43)
 27944 Biotechnology and process design (29) (B)
 31525 Physiological transport phenomena (12)
 41683 Materials Science (30) (B)

EDUCATION CONTINUED

MASTER'S AND BACHELOR COURSES

FALL SEMESTER

28001 Introduction to Chemistry and Chemical Engineering (63)
28012 Chemical and Biochemical Process Engineering (42) (B)
28016 Mathematical models for chemical and biochemical systems (26) (B)
28022 Unit Operations of Chemical Engineering and Biotechnology (37) (B)
28121 Chemical Unit Operations Laboratory (20)
28140 Introduction to Chemical Reaction Engineering (33)
28150 Introduction to Process Control (35)
28156 Process and product design (27) (B)
28213 Polymer Technology (33)
28233 Recovery and Purification of Biological Products (40)
28242 Chemical Kinetics and Catalysis (49)
28244 Combustion and High Temperature Process (75)
28246 Applied Enzyme Technology and Kinetics (35)
28247 Advanced Enzyme Technology (12)
28310 Chemical and Biochemical Product Design (35)
28315 Colloid and Surface Chemistry (40)
28316 Laboratory Course in Colloid and Surface Chemistry (11)
28322 Chemical Engineering Thermodynamics (24) (B)
28342 Chemical Reaction Engineering (28) (B)
28352 Chemical Process Control (22) (B)
28361 Chemical Engineering Model Analysis (24)
28420 Separation Processes (33)
28515 Enhanced Oil Recovery (19)
28530 Transport Processes (33)
28811 Polymers in Processes and Products (9)
28845 Chemical Reaction Engineering Laboratory (20)
28864 Introduction to Matlab Programming (34)

Courses given in cooperation with other departments:

10336 Fundamentals Problems in Fluid Dynamics (11)
26010 Introductory Project in Chemistry (41)
27004 Health, Diseases and Technology (56)
27944 Biotechnology and process design (22) (B)
41657 Materials Science for Chemists (44)
41683 Materials Science (23) (B)

MASTER OF SCIENCE DEGREES

59 students finished their research projects for the MSc degree. The project titles and names of the students are listed below:

Akbas, Erkan and Suzan Sager Hassouneh
Microstructuring of Elastomer Films

Andersen, Christian Kjeldgaard
Characterization of SOEC for Production of CO, H₂ and Syngas

Ballesteros Fernandez, Elena
Separation of azeotropic mixtures

Bartholdy, Sofie Holme
Modeling of adsorption on molecular sieves and silica gel using the Ideal, Real Absorbed Solution and Langmuir theories

Bisgaard, Thomas
Dynamic effects of diabatisation in distillation columns

Bjørner, Martin Gamel
Modeling of adsorption on molecular sieves and silica gel using the Potential Adsorption Theory

Buckland, Peter William
Evaluation and Application of Factorial Design in the Development of a Production Process for a Pharmaceutical Product

Christensen, Kim Müller
Sulphur emissions from Cement Production

Dode, Sharad Suryakant
Process Analytical Technology (PAT): Implementing and Testing Sensor Models for Realistics Simulation of Control Strategi

Dudus, Senol
Release of Inorganic Matter during Biodust Combustion

Duranni, Adam
Towards an integrated microfactory: Rapid prototyping for an experimental investigation of a miniaturized reactor for biocatalysis

Eisenhardt, Kristian Hedberg
Amino acid salt solutions for CO₂ capture

Engelbrechtsen, Mette
Evaluation of Bio-derived catalysts for pretreatment of lignocellulosic biomass

Eriksen, Daniel Kunisch
Towards the development of a polar CPA equation of state

Eriksen, Winnie Laurentzius
Synthesis and characterisation of CuNi based catalysts for methanol synthesis

Graversen, Mia Boesgaard
Segregation of particulate solids

Halaburt, Birgitte Louise
Homogeneous oxidation of CS₂, H₂S and H₂S/CS₂ mixtures

Hallas-Møller, Magnus
Enzymatic modification of bran: Kinetics and mechanisms

Hansen, Bjørn Bredgaard
Release for inorganic elements in bio-dust combustion

Hansraj, Sterlin
Catalytic deoxygenation of biooil

Hauksdottir, Katrin
Rheological characterization of Hyaluronic and solutions

Heintz, Søren
Cake Compaction and Drying Studies for Optimization of Decanter Centrifuges Used for Enzyme Recovery

Hendriksen, Simon Bach
Mixing of particulate solids

Hugelier, Siewert
Mass transfer in stirred microbioreactors

Ibrahim, Hulouvan Kamal
Solid-liquid separation processes in the pharmaceutical industry

Jensen, Johan Bruun
Enzymatic Hydrolysis of Cellulose in Biomass: Reaction Kinetics for High Extents of Conversion

Jensen, Paw
Combustion and modelling of alternative fuels

Jespersen, Jacob Boll
Sulfate additives for KCl control in biomass combustion

Jiang, Yu
Epoxy-based Anticorrosive Coatings for High Temperature Conditions

EDUCATION CONTINUED

MASTER OF SCIENCE DEGREES CONTINUED

Kadhim, Adam Samir

Optimization of industrial crystallization process

Kart, Turgay

Optimization of Industrial Crystallization Process

Krüger, Thomas Christian

Modeling the conductivity of salt solutions

Lopez Garcia, Javier

Chemometric Determination of Enzyme Kinetics

Lopez Torres, Santiago

Characterization of Beta-galactanase

Lykkestrup, Merete

Optimizing the pectin extraction

Madsen, Kasper Rich

Enzymatic Modification of Bran: Mechanism and Functional Effects

Mestres Rosás, Arnau

Characterisation and Parametric Study of the Flow Properties of Cohesive Powders at Temperatures up to 850oC

Meyland, Lene Have

Process modelling and design for enzymatic biodiesel production using lipases

Munk, Line

Effects of Oxidative Enzymes on Insoluble Cereal Substrates

Münther, Anette Ulla

Optimization of Cement Clinker Burning

Møller, Michala Karlsen

Economic feasibility study of biorefineries

Nielsen, Jacob Clement

Production of synthesis gas by electrolysis of carbon dioxide and water

Nielsen, Jan Erik

Diabatic Distillation

Nordby, Mads Willemoes

Interactions between CO₂ and SO₂ capture in carbonate looping applied to cement industry

Nordvang, Rune Thorbjørn

Cloning of Genes in Starter Cultures

Pedersen, Anders Kristian

Enzymatic pre-treatment of low-grade feedstock oil for biodiesel production

Pennati, Alessandra

Synthesis of Water Networks

Petersen, Thomas

Freeze drying: Computational Fluid Dynamics and experiments

Poehler, Annalicia Camilla

Continuous crystallization in the pharmaceutical industry

Seerup, Rasmus

Towards an Integrated Microfactory: Detailed Investigation of Material Characteristics in a Microfluidic System

Sengeløv, Louise With

HCl emissions from modern cement production processes equipped with a by-pass

Svanholm, Frederik Dalgaard

Cross-Linking Chemistry Kinetics for Production of Immobilized Enzymes

Swiniarska, Malgorzata Maria

New Hydrolases from Filamentous Fungi

Sønderby, Tim Lyng

Computational Fluid Dynamics modelling of an 80 L bioreactor

Therkelsen, Niels Peter Vegger

Methods to determine the efficiency of nozzles for cleaning process equipment

Thorsen, Kristian

Biological Activities of Prebiotic Oligosaccharides

Valverde Perez, Borja

Advanced process control for innovative nitrogen removing processes

Zhou, Guofeng

Model Based Control and Monitoring of the SCR Process for Diesel Engines

BACHELOR OF ENGINEERING DEGREES

21 students finished their research program for the BEng degree. The project titles and names of the students are listed below:

Andersen, Hans Erik Samuel and Kristian Karlsen

Synthesis of methane from carbon dioxide and hydrogen

Berner, Micha

Optimization of silicone coatings for biofouling control

Falkesgaard, Mette Hvas and Majken Jessen

Emissions from Wood Stoves with automatic control systems

Filimon, Vasile Jensenius

Measurement of Oil-water Contact Angles on Mineral Surfaces

Flensburg, Julie Pauline

Release of K, S, and Cl during Pyrolysis of Biomass

Grave, Rikke Mia

Synthesis and Characterization of Hydrophilic Polyurethane Foam using Isocyanate-terminated Pre-polymers

Hejselbæk, Jesper Kailow

FT-NIR calibration and in-line implementation for quantification of wort constituents in large scale brewing

Ishøy, Jonas

Modelling of sulphuric acid catalysts under transient conditions

Jensen, Morten Walk

Homogeneity and vitality investigation of yeast mixing

Jensen, Susanne Helene

Anisotropic polymer films

Jørgensen, Rasmus Dan

Evaluation of Novel Reactor Technology for Enzymatic Biodiesel Production

Larsen, Jacob Seneca

Oxidation of Elementary Mercury by Bromine over SCR Catalysts

Mahmood, Zulqurnain

Selfhealing Anticorrosive Coatings

Nielsen, Henrik Lund

Design, simulation, and energy optimization of CO₂ reduction process using amino acid salt solutions

Prior, Rasmus Andreas and Tobias Vilby

Validation of 2 mL Microbioreactors and Near-infrared Spectroscopy Monitoring

Storgaard, Thomas Busch

Anticorrosive coatings and underfilm corrosion

Sørensen, Helena

FT-NIR and FT-IR calibration and in-line implementation for quantification of wort constituents in laboratory and pilot scale brewing

Wiebe, Maria Meldgaard

Packaging Material Film with Perforations: Feasibility Study of Temperature-controlled Oxygen Permeation in Plastic Pack





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.....
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Student Committee

Staff

Industrial PhDs and Guests

The Faculty

Departmental Seminars 2012

ADVISORY BOARD



LARS BANG

SENIOR VICE PRESIDENT, SUPPLY OPERATIONS & ENGINEERING · H. LUNDBECK A/S

Scientific research at university level is a prerequisite for the development of Lundbeck's chemical activities in Denmark. We have had a beneficial cooperation with DTU Chemical Engineering for several years, collaborating on PhD projects and recruiting several of its candidates. Furthermore, it has been a great advantage to be able to draw on the knowledge of DTU Chemical Engineering's scientific staff as advisors/consultants.



KIM PANDRUP CHRISTENSEN

EXECUTIVE VICE PRESIDENT · ANDRITZ FEED & BIOFUEL A/S

The close cooperation with DTU Chemical Engineering has ensured significant results within the biofuel technology which will benefit a lot of industries. Long-term focus on development and innovation is necessary to meet the ever changing opportunities, rules, legislation and profitability demands that all industries are faced with. DTU Chemical Engineering ensures a high level of education, motivated candidates and industrial cooperation in important research projects that will lead to technologies of the future.”



BJERNE CLAUSEN

PRESIDENT AND CEO · HALDOR TOPSØE A/S

Working closely with the best research groups within the fields of our core competences is of major importance to Haldor Topsoe A/S. Our cooperation with DTU Chemical Engineering enables us to resolve research challenges beyond our competences and resources and is an important source of inspiration and knowledge for employees at Haldor Topsoe, benefiting their own and the company's development.



PEDER HOLK NIELSEN

EXECUTIVE VICE PRESIDENT · ENZYME BUSINESS · NOVOZYMES A/S

At Novozymes we see innovation-driven partnerships as a key element in delivering tomorrow's solutions. At university level we have had an exemplary cooperation with DTU Chemical Engineering for many years. This cooperation supports and complements our efforts in developing and testing new technologies, attracting new valuable employees and driving the world towards sustainability. DTU Chemical Engineering fully answers these demands.

STUDENT COMMITTEE



KTStudents is the student organization at DTU Chemical Engineering. KTStudents seek to provide engineering and non-engineering related activities for students that are part of or affiliated with the department. These activities span over a wide range and include:

1. Company and Technical Presentations – companies are invited to present an overview of their work and a technical lecture so the attending students have an idea of the type of R&D or engineering tasks faced at the company

2. Company Trips – company sites are visited by the students. These events are normally fully funded by the companies themselves and the companies typically have production or pilot facilities which give students an image of the real world

3. Social Events – The goal of these are to give students the opportunity to socialize and net-work with other students whom they would otherwise be unable to meet during the hectic semester

4. Research Opportunities – This has been held by KTStudents for the past two years. The 7 research centers at the department present research opportunities at their centers ranging from BSc over MSc to PhD projects

5. Roundtable discussions – This has been held jointly with the department the last two semesters. When a leading researcher visits the department, the students have an exclusive opportunity to meet the researcher and discuss a wide range of topics

In November 2010, KTStudents became the 1st student chapter in Europe to house an American Institute of Chemical Engineers (AIChE) Student Chapter. The AIChE is the largest society for chemical engineers, offering technical information and networking for studying and practicing chemical engineers.

KTStudents continues to expand with an ambitious plan in 2013 to hold our first annual one-day student conference where students from the BSc and MSc levels will have the opportunity to present their research and projects at oral and poster sessions.

Asbjørn Toftgaard Pedersen, President, KTStudents

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Deputy Director



Gunnar Jonsson
Associate Professor



Sten Bay Jørgensen
Professor Emeritus



John Villadsen
Professor Emeritus

DEPARTMENTAL SEMINARS AT DTU CHEMICAL ENGINEERING IN 2012

JANUARY 31

Dr. Ryan L. Hartman, University of Alabama, USA

"Engineering Heterogeneous Reactions in Micro-scale Laminar Flow for Fine Chemicals Processing"

FEBRUARY 28

Senior Scientist Constance Senior, ADA Environmental Solutions, USA

"Behavior of Trace Elements in Combustion Systems"

APRIL 12

Associate Professor Shelley S. Anna, Carnegie Mellon University, USA

"Interfacial Transport and Mechanics at the Microscale"

MAY 15

Dr. Jan Pfeffer, Evonik Industries AG, Germany

"Conversion of Renewable Raw Materials into Fine Chemicals"

JUNE 14

Dr. Simone Bastianoni, University of Siena, Italy

"To Be or Not To Be... Sustainable"

SEPTEMBER 13

Dr. Jeffrey J. Siirola, Purdue University & Carnegie Mellon University, USA

"Thoughts on Sustainability, Energy, Renewable Resources, and Shale"

OCTOBER 4

Tony Moorwood, Infochem Computer Services Ltd., UK

"Physical Property Modelling - The Commercial Point of View"

NOVEMBER 7

Professor Jörg Hübner, Director DTU Danchip, DK

"Research collaboration with DTU Danchip"

NOVEMBER 29

Professor Steven Holdcroft, Simon Fraser University, Canada

"Nano-Scale Morphology and Conductivity of Proton Conducting Membranes"



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USEFUL INFORMATION

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- Department of Chemical and Biochemical Engineering
- Departments
- Oticon Hall
- Administration
- Campus Service
- Residential halls and guest houses
- Scion DTU
- Instructional buildings
- Bus stops
- Canteens
- DTU Library
- DTU Meeting Center







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