**NTNU**
**Norges teknisk-naturvitenskapelige universitet**

**Fakultet for naturvitenskap og teknologi**
**Institutt for kjemisk prosessteknologi**

# Forslag til masteroppgaver våren 2011

# ved

# Institutt for kjemisk prosessteknologi

## Fagområder/-groups:

1: Katalyse / Catalysis Group
2: Kolloid- og polymerkjemi / Colloid- and Polymer Chemistry Group
3: Miljø- og reaktorteknologi / Environmental Engineering and Reactor Technology Group
4: Prosess-systemteknikk / Process Systems Engineering Group
5: Bioraffinering og fiberteknologi / Biorefining and fibre technology

# Katalyse/Catalysis Group

## AH: Professor Anders Holmen

**AH-1: Hydrothermal synthesis of cobalt Fischer-Tropsch catalysts with implications on chemical attrition and syngas conversion.**
***Supervisors: Anders Holmen, Erling Rytter.***
***Reserved for Aina-Elin Karlsen.***

**AH-2. Conversion of synthesis gas on iron Fischer-Tropsch catalysts.**
***Co-supervisors: Andreas Helland Lillebø, Bjørn Christian Enger.***
***Reserved for Claire Barilleau***

**AH-3: EDC cracking – microkinetic modeling**
We have previously studied cracking of EDC (ethylene dichloride) in the laboratory. We are now planning to use these results to develop a microkinetic model that can be used to describe the results. The main reactions take place in the gas phase, but the interplay between surface reactions and gas phase reactions are also important and the model should therefore describe the surface reactions as well as the gas phase reactions.
***Co-supervisor: De Chen.***

**AH-4: Catalytic partial oxidation of methane at moderate temperatures**
The work will focus on preparation of new catalysts, on characterization of the catalysts (by use of TPO, chemisorption, BET) and on testing of the catalysts. The work will include the stability of nanocomposites of the type $Zr_x$, $Ce_{1-x}O_2$ $Al_2O_3$ as well as the use of inactive aluminate spinels as precursors for partial oxidation catalysts.
***Co-supervisor: Bjørn Christian Enger***

## EAB: Professor Edd A. Blekkan

**EAB-1: Catalytic reforming of producer gas from biomas gasification**
***Veiledere/Supervisors: Edd A. Blekkan, Espen S. Wangen.***
***Reserved for Katrine S. Biesterfeld Plünnecke***

**EAB-2: Catalytic dehydrogenation of propane**
The catalytic dehydrogenation of propane is a very demanding process designed to overcome the thermodynamics of the main reaction (strongly endothermic and equilibrium limited). Furthermore the reaction conditions are such that coke formation is an important issue. We work on an alternative process concept, where the idea is to add some oxygen to the system, selectively burning approximately 50% of the hydrogen produced, thus providing in situ process heat, and at the same time removing some hydrogen and "pulling" the equilibrium conversion towards the product side. A key issue is finding a catalyst capable of burning only the hydrogen in a stream also containing reactive hydrocarbons. The project will involve experimental and theoretical investigations of the selective hydrogen combustion, developing a catalyst system for this demanding process. The work will include a literature review, catalyst preparation and characterization, and testing in a dedicated experimental set-up.
***Supervisors: Edd A. Blekkan, Ilya Gorelkin***

## DC: Professor De Chen

**DC-1: Synthesis and applications of nanoparticles with different sizes and shapes**
Nanotechnolgy deals with exploring novel properties (e.g. electrical, physical, chemical) that occur at the nanoscale level to create structures (e.g. functional materials, devices, or systems) atom by atom. Building nanoarchitectures by controlling atomic assembly to achieve manipulating material properties has opened a

great opportunity for improving catalyst activity, selectivity and stability. Nanosized catalyst constituents are important for functions that require structural control over several scales of dimension. Nanaocatalysis plays an important role in sustainable development of society. The project work includes synthesize metal and metal oxide nanoparticles with well controlled sizes and shapes and surface compositions. The materials will be characterized by different techniques and tested in propane dehydrogenation in a fixed bed reactor or PEM fuel cells.

***Co-upervisors: Dr. Jun Zhu, PhD Navaneethan Muthuswany***

## DC-2: Kinetic study of oxychlorination process

Catalytic oxychlorination of ethylene with hydrochloric acid and oxygen is the important industrial process to produce 1,2-dichloroethane, which can be converted into vinyl chloride cracking. Supported $CuCl_2$ catalyst often used as oxychlorination catalysts. The present work focus on the catalyst preparation and characterization of $CuCl_2$ layer on alumina supports. The site reactivity will be studied by UV-Vis spectroscopy and transient kinetic study on catalyst with different site density.

***Co-supervisor: Miroslave Surma***

## DC-3: Kinetic study of high temperature water gas shift reaction

High temperature water gas shift reaction is crucial for produce high purity hydrogen from different compounds such as natural gas and biomass derived polyols by sorption enhanced reforming. The present work deals with catalyst preparation and characterization of hydrotalcite derived Ni and Co mixed catalysts. Detailed kinetic study will be performed to elucidate reaction mechanism of water gas shift reactions at high temperature (400-650 ◦C).

***Co-supervisor: Tayyaba Noor***

## DC-4: Sorption enhanced reforming

Sorption enhanced reactions including sorption enhanced reforming is a promising process to overcome the thermodynamic constrains and to reach one-step hydrogen production with high purity and yield. The $CO_2$ high temperature acceptors and catalysts are installed together in the reactor. The present work will focus on the fundamental understanding of in-situ remove on the surface reactions on Ni surfaces through a detailed kinetic study.

***Co-supervisor: Saima Sultana Kazi***

## DC-5: Catalysis in conversion of biomass to fuels

Catalysis plays a very important role in conversion of biomass to liquid fuels, which becomes an important alternative to supply renewable fuels in future energy system. There are many reaction routes to convert biomass to fuels, which can be classified into two categories, namely indirect route through gasification and direct route through sugar-based building block. The Department of Energy (DOE) has identified the twelve sugar-based building blocks such as 1,4-diacids (succinic, fumaric and malic), 2,5-furan dicarboxylic acid, 3-hydroxy propionic acid, aspartic acid, glucaric acid, glutamic acid, itaconic acid, levulinic acid, 3-hydroxybutyrolactone, glycerol, sorbitol, and xylitol/arabinitol for production of biomass bassed high value chemicals and materials. The present work will analyze different building blocks and catalysis for production of gasoline and diesel fuels from biomass by a detailed literature study. Develop of new metallic catalysts for conversion of selected building block to gasoline and diesel will be the part of the project work and the main objective of the diploma work.

## DC-6: Synthesis and applications of nanomaterials in clean energy

Carbon nanotubes (CNT), especially aligned CNT arrays have long studied for their potential applications in catalysis as well as energy production, storage and utilization. They present a great interest as electrodes for many applications including fuel cells, solar celles, photoelectrochemical cells and chemical/biological sensing, and they play an increasing role in energy storage, particularly in electrochemical supercapacitors for high power and high energy density applications. The outstanding properties of individual CNT and their anisotropic structure make aligned CNT based nanoelectrode arrays, where each individual CNT serves as a nanoelectrode, promising for many applications. Moreover, the high reactivity of CNT surfaces makes it possible to fabricate diverse hybrid nanoeletrode arrays by coupling different functional materials in or on CNT, such as conductive polymers, semiconductor clusters including quanta dots, and metal

clusters. The project work will include synthesis of aligned CNT on different metal foils as the core, and deposit second materials as the shell by chemical or electrochemical method. The materials will be characterized by different techniques. Tow projects are proposed here based on nanoelectrode array as a platform with different applications:
Conductive polymer-CNT array will be used as electrodes in super capacitors with high power and energy density. The electrode will be tested in electrochemical station as supercapacitors.
Or: Semiconductor-CNT array will be tested as electrodes in photoelectrochemical cell for ethanol reforming.
***Co-supervisors: Fan Huang, Dr. Estelle Vanhaecke, Prof. Magnus Rønning***

## *MR: Professor Magnus Rønning*

### MR-1: Water purification by using structured catalysts for hydrogenation of nitrates

The increasing concentration of nitrates in the ground water and the increasingly more rigorous quality standards for water purification generate the urgent need to develop an improved technology for the removal of nitrates from aqueous solutions. This demand is reflected within the $7^{th}$ framework of the European Community, where sustaining the quality of the earth's water resources is one of the major objectives. During the last years, especially in agricultural areas, a steady increase of nitrate concentration in the water from the intensive use of natural and synthetic fertilizers can be observed. The concept of the project is the development of an emerging technology for the catalytic detoxification of water. This technology is based on the development of structured reactors for the purification of aqueous effluents using catalytic processes. The work will involve catalyst development and characterisation and kinetic studies in a reactor system for liquid phase hydrogenation of nitrates using $H_2$ over bimetallic catalysts (Cu-Pd/carbon). The work is part of a European FP-7 funded project and is a collaboration with academic and industrial partners from several European countries.
***Supervisor/ co-advisor: Magnus Rønning/ Estelle Vanhaecke***
***The project is reserved for Kimete Osmani***

### MR-2: Photocatalytic fuel production through splitting of water and phororeforming of hydrocarbons

Producing hydrogen from photocatalytic water splitting and photoreforming of hydrocarbons is an emerging field within renewable energy research. Photocatalysts that can operate at ambient temperature without producing harmful by-products are ideal as environmentally sound catalysts. For such systems to be considered in large-scale applications, photocatalytic systems that are able to operate effectively and efficiently not only under UV light, but also under sunlight must be established. The project involves synthesis and characterisation of efficient materials for photocatalysis and testing of the catalyst materials in photocatalytic reactions. The work will concentrate on photoreforming of alcohols in a batch reactor set-up using Cu-$TiO_2$ catalysts.
***Supervisor/ co-advisors: Magnus Rønning/ Asmira Delic/ Charitha Udani***
***The project is reserved for Ida Lien Bjørnstad***

### MR-3: Characterisation of promoted Fischer-Tropsch catalysts

*In situ* characterisation methods are able to give information about catalysts and catalytic reactions at reaction conditions close to industrial processes. The Catalysis Group is using an increasing number of advanced *in situ* techniques for catalyst characterisation. Accessible techniques are spectroscopic techniques such as Raman, IR and UV-vis. The project deals with *in situ* Raman, IR and XRD studies of Fischer-Tropsch catalysts at industrially relevant conditions in terms of pressure, temperature and feed composition. The work will include synthesis of promoted catalysts and exploration of new experimental methods, optimisation and data analysis. The project will be carried out in association with InGAP, a recently awarded centre for research based innovation, and in close collaboration with Statoil and SINTEF.
***Supervisor/ co-advisor: Magnus Rønning/ Alexey Voronov/ Georg Voss***
***The project is reserved for Vegar Evenrud***

### MR-4: New catalysts for preferential oxidation of CO in presence of hydrogen (PROX)

Small amounts of carbon monoxide may have detrimental effect on the PEM fuel cell anode activity. Hence, the CO concentration in the hydrogen feed to PEM fuel cells should be kept well below 100 ppm. Purification of hydrogen from reformed hydrocarbons can be obtained by the water-gas shift reaction followed by preferential oxidation of CO (PROX). This project deals with synthesis and characterisation of new Cu-based catalysts on various oxide supports. Potential characterisation methods are chemisorption, TGA/DSC, XRD, TEM/SEM and vibrational spectroscopy. The catalysts will be tested in the PROX reaction using a fixed-bed reactor.

***Supervisor/ co-advisors: Magnus Rønning/ Nina Hammer***

## *HJV: Førsteamanuensis Hilde J. Venvik*

### HJV-1: Bifunctional catalyst for the direct DME synthesis.

Dimethyl ether (DME), $CH_3OCH_3$, is the simplest ether and a possible clean and economical fuel for the future, with characteristics as a sulfur free diesel fuel with low particulate emissions and high cetane number. The properties of DME are similar to those of LPG and it can hence be used for power generation as well as residential heating and cooking. DME is currently produced in a two-step process; a methanol synthesis step followed by the methanol dehydration reaction. In order to use DME as a fuel, it must be produced at low cost in large quantities. The catalytic dehydration of methanol is carried out over an acidic catalyst, and the cost of producing DME from methanol is influenced by price and availability of methanol. DME production from syngas is thermodynamically more favourable than from methanol and the direct DME synthesis should thus be more economic, provided a suitable catalyst is identified and combined with the appropriate reactor technology. The project includes the synthesis, characterization and testing of catalysts for the direct DME synthesis, for which a state-of-the art experimental set-up has been built. The MSc project focuses on comparing the functionality of the bifunctional catalyst in the direct synthesis from synthesis gas to that in the methanol dehydration.

***Co-advisors: Prof. Anders Holmen, PhD student Fatemeh Hayer.***

### HJV-2: Kinetics and deactivation in the methanol synthesis reaction.

The methanol reaction is a highly exothermic reaction that takes place over a catalyst at 200-300C and elevated pressure. New reports claim enhanced selectivity and productivity of the reaction in so-called microchannel reactors, utilizing the enhanced heat and mass transport properties of the microchannel systems, and it is the objective of an ongoing PhD project to assess this potential. The kinetics of the methanol synthesis has been much studied and reported in the literature. The project will establish whether kinetic data obtained in the microchannel reactor are in line with previous reports or whether a further improved understanding can be obtained. Kinetic modelling can be part of this task. The MSc project will further address the deactivation mechanisms of the methanol synthesis catalyst in the microchannel reactor.

The project is part of a collaboration with SINTEF Materials and Chemistry.

***Co-advisors: Prof. Anders Holmen and Rune Myrstad (SINTEF)***

### HJV-3: Microchannel membrane reactor for small scale hydrogen production

Membrane reactors combine separation and reaction in a single step. The yield of a product may also be increased by its extraction through the membrane if the reaction is equilibrium limited. Palladium based membranes are 100 % selective to hydrogen and hence suited for reactions that produce hydrogen, such as steam reforming of methanol methane, or the water-gas shift (WGS) reaction. A possible application is miniaturized production of hydrogen for fuel cells, as an alternative to batteries. Promising results were recently obtained by integration of thin (<5μm) Pd membranes developed and patented by SINTEF Materials and Chemistry into a microchannel geometry.

We recently showed that the membrane's sensitivity to carbon monoxide (CO) could be changed (reduced) through a particular heat treatment, which has important implications for their applicability. The microchannel configuration is particularly suited for investigations of the phenomena that give this change.

The topic involves studies of the effect of CO and $CO_2$ in the membrane microchannel configuration through experiments and modelling, as well at characterization of surface species present on the membrane during and after permeation experiments. A next step will then be to approach methane steam reforming conditions. The work will be carried out in collaboration with SINTEF Materials and Chemistry in Oslo.
***Co-advisor: Thijs Peters (SINTEF), PhD student Nicla Vicinanza, Post doc. Ingeborg-Helene Svenum.***

# Kolloid- og polymerkjemi/Colloid- and Polymer Chemistry

## *JOHS: Professor Johan Sjöblom*

### JOHS-1: Rheological Model Development

Rheometric experiments will be performed to establish the time-dependency of the local stress tensor $\tau_{zz}$ which describes the breakdown of a wax-gel. Initially, experiments will be performed in a shearing rheometer. If necessary, experiments will also be performed in an extensional rheometer. Various literature models to describe the local gel breakdown kinetics will be investigated, and if necessary, a new breakdown model will be proposed and developed.

The rheological model will yield fundamental knowledge of the local gel breakage mechanism. The influence of the following factors on the stress tensor $\tau_{zz}$ will be investigated:

- Shear, Time, and Thermal History
- Wax Amount, Wax Carbon Number Distribution, and Wax Molecular Structure
- Other Colloidal Fractions such as Asphaltenes and Resins
- The Presence of Water and Gases
- Initial Oil Viscosity
- Additives

The rheological model will be tested starting with simple model fluids consisting of refined paraffin wax dissolved in mineral oil. Both micro-crystalline and macro-crystalline waxes will be blended into the model fluids in order to gauge the effect of paraffin molecular structure on gel strength. Subsequently, other oil components such as asphaltenes, resins, water and gases may be added to understand the influence of oil composition.

***Co-supervisor: Kristofer Paso***

### JOHS-2: Emulsion Separation Modeling

The separation of emulsions is a critical phenomenon in a myriad of industries ranging from food and cosmetics to chemicals and petroleum. Modeling the mechanisms of emulsion separation and quantifying the interplay of these mechanisms to establish a fundamental theoretical framework is a research task of great importance to both industry and academics. The focus of this project is to employ the population balance model for emulsion separation developed at Ugelstad Laboratory to investigate various interfacial phenomena on the behavior of emulsion separation. Focus will be place on hindered settling of poly-disperse emulsions, incorporating the local mass balances of surface active compounds, and relating these phenomena to the formation of dense packed emulsions. The student will also be familiarized with the various experimental techniques employed to measure the evolution of the dispersed phase in separating emulsions as well as experimental techniques employed to characterize interfacial phenomena. The project incorporates a broad spectrum of chemical engineering topics including mass transport, momentum transport, thermodynamics, and colloid chemistry thereby providing the student with a glimpse of how these topics are interrelated in real chemical processes important to industry. This project is supported by an industrial consortium of about a dozen major oil and oil service companies and the student will be expected to meet and present their work to the industrial consortium.

***Co-supervisor: Brian Grimes***

## *GØ: Professor Gisle Øye*

### GØ-1: Preparation and characterisation of superhydrophobic surfaces

Superhydrophobic and self-cleaning surfaces play an important role in many technical applications, including coatings for antifouling and drag reduction of fluid flow in microchannels. The master project focuses on preparing hierarchical superhydrophobic surfaces. The surface properties will be characterised

by SEM and wettability measurements, while the mechanical durability will be measured by AFM. The project will be carried out at NTNU Nanolab and Ugelstad Laboratory
***Supervisor: Gisle Øye (gisle.oye@nt.ntnu.no)***

### GØ-2: Advanced characterisation of produced water

Produced water is an increasing challenge during production of oil and gas. Water co-produced with crude oil often contain a significant proportion of dispersed components (particles, oil and gas) which must be removed before the water is recycled in the process or discharged to sea. Consequently, it is important to improve existing and develop new treatment technologies for produced water. This requires fundamental understanding of the fluids. The master project will focus on experimental characterisation of particles at oil-water interfaces, with the aim to better understand how particles can stabilise oil-in-water emulsions. Important parameters will be the chemical composition of particles, water and crude oil.

The project will be carried out at Ugelstad Laboratory, and is a collaborative project with ConocoPhillips, Statoil and Total.
***Supervisors: Bartlomiej Gawel and Gisle Øye***

## *WRG: Førsteamanuensis Wilhelm R. Glomm*

### WRG-1: Protein-nanoparticle constructs for intracellular delivery

**Background:**
Interaction of dissolved proteins with nanomaterials and interfaces is essential for a wide range of applications, ranging from reduction of biofouling via biosensing and enzymatic catalysis to targeted intracellular drug delivery. An understanding of the underlying mechanisms and interaction kinetics is therefore crucial to the design of new smart materials which can be used to control protein deposition and delivery. Protein-surface and protein-protein interactions are determined by chemical and physical factors such as electrostatic forces, curvature and size, hydrophobic interactions and steric constraints. This in turn leaves an abundance of possibilities for manipulation of relevant surfaces, enabling interaction studies with biological membrane mimics and various delivery vehicles (e.g., Au nanoparticles, liposomes).

In this project, the interaction and interfacial activity of protein-modified nanoparticles will be investigated using experimental techniques available at the Ugelstad Laboratory (spectroscopic techniques and interfaceial measurements) as well as in the NTNU NanoLab (NanoSight, AFM). The project is suitable for one or two students.
***Main subject teacher: Wilhelm Glomm, IKP, e-mail: glomm@nt.ntnu.no, Phone: 73 59 41 58***
***Co-supervisors: Sondre Volden, Sina Maria Lystvet (IKP)***

### WRG-1: Carbon nanotubes in polymer composites

The properties of polymeric materials are tunable via addition of different types of nanostructures, such as nanoparticles nanofibers and nanotubes. Thus, plastics, composites or adhesives with improved properties can be manufactured using nanotechnology. A lot of research is being done on the development of lightweight materials with extreme mechanical properties, particularly within the aviation, missile and space industries.

In this project, the main focus will be on the change in mechanical properties of a polymer upon addition of nanofibers – higher tensile strength and stiffness being target variables. The change in these target variables are investigated via mechanical testing of the resulting polymer composites. An important subgoal is to understand why the addition of carbon nanotubes leads to improved mechanical properties, and which mechanisms govern these changes. The application of microscopy (TEM, SEM and AFM) will be esssential tools by which to investigate these systems.

The project will be a part of a larger effort at the Norwegian Defence Research Establishment (Forsvarets Forskningsinstitutt, FFI), where the main objective is modelling and characterization of the mechanical properties of nanocomposites.

***Main subject teacher: Wilhelm Glomm, IKP, e-mail: glomm@nt.ntnu.no, Phone: 73 59 41 58***
***Co-supervisor: Bernt B. Johnsen (e-post: bernt.johnsen@ffi.no)***

## WRG-1: Interfaces in composite materials – effect of nanoparticles

Composite materials are much used e.g. in aviation, missile and space industry, as they are light-weight materials with extremely desirable mechanical properties, which can be tuned to specific applications. In these composite materials, fibers provide the materials strength, while the polymer is mainly used as a matrix in which to disperse the fibers. Use of nanotechnology, for example via addition of nanotubes or various kinds of nanoparticles to the polymer matrix, opens up new possibilities for improvement and tunability of the fiber composite properties.

The main objective of this project is to investigate the polymer/fiber interface, specifically how inclusion of fibers in the polymer matrix affects the interfacial properties. Interfacial properties (*i.e.*, structure) and how these ultimately affect mechanical strength will be investigated via experimental techniques such as microscopy (SEM, TEM and AFM) and mechanical testing. The project will be carried out in close collaboration with the Norwegian Defence Research Establishment (Forsvarets Forskningsinstitutt, FFI).

***Main subject teacher: Wilhelm Glomm, IKP, e-mail: glomm@nt.ntnu.no, Phone: 73 59 41 58***
***Co-supervisor: Bernt B. Johnsen (e-post: bernt.johnsen@ffi.no)***

# Prosess-systemteknikk/Process Systems Engineering

## SiS: Professor Sigurd Skogestad

### SIS-1: Simulation and operation of $CO_2$ capturing process

There are many possibilities for capturing $CO_2$ in combustion processes. We have previously considered conventional atmospheric post combustion $CO_2$ capture, but in this project other alternatives will be studied. The goal is to study the dynamics and optimal operation of the process using the ProSim (Hysys) dynamic simulator. The operational profit to be maximized is income from $CO_2$ removal minus the energy costs. It is desired to find a simple control strategy by identifying "self-optimizing" controlled variables, which when held constant indirectly maximize the profit.

***Co-supervisor: PhD student, Mehdi Panahi***

### SIS-2: Simulation, design and optimal operation of liquefaction process for natural gas

LNG (Liquefied natural gas) is still a growing business, both in Norway and abroad. Liquified natural gas (LNG) is produced by cooling natural gas in several stages to about -162C so that it can be stored as liquid as atmospheric conditions. The volume is then reduced by a factor of about 600. The process is energy and capital intensive and many alternative designs have been proposed. The basis for the project are existing models of the process in Hysys/Unisim , MATLAB or gPROMS.

2.1: Steady-state simulation and optimization of LNG processes is difficult because of tight integration and small temperature differences between the streams.
The UniSim and gPROMS models use different solution procedures, but both programs have problems in converging. In this project the focus is on formulation robust model approaches by combining the best from the UniSim and gPROMS models.

2.2: In this project the focus will be on processes that take advantage of arctic temperature conditions.

***Co-supervisor: Magnus G. Jacobsen***
***The projecta will be in cooperation with Statoil (Jostein Pettersen)***

### SIS-3: Design of integrated distillation columns for separation of multicomponents mixtures

3.1: **Integrated Process Design.** Integrated (simultaneous) design is defined as the development of a chemical process by considering both steady-state economics and dynamic controllability at all stages of flowsheet synthesis. The basic notion is that the dynamics of the process are vitally important in its ability to operate efficiently and safely and to make on-specification products with little product-quality variability.
First, the need of simultaneous consideration of design and operation and the conflicts between steady-state economics and dynamic controllability will be studied. Afterwards, a good process design and control structure design will be done considering the steady state objectives and good controllability performance.
The model is provided is UniSim/HYSYS and the tool for manipulating the HYSYS model and doing the rest will be in MATLAB.

3.2: We have worked for many years on new integrated distillation sequenses, including Petlyuk distillation and the Kaibel column.
More specifically, the goal of this project is to look for the optimized thermally coupled distillation sequences for multi-component separations. A rigorous model is developed in

UNISIM and MATLAB or GAMS will be used for the optimization. So, the capabilities of both software systems are used at the same time. Different alternatives are simulated in UNISIM and then the best option should be selected considering the energy savings through a proper optimization of the interconnecting streams.

3.3: Comparison of two plant-wide control strategies for the case of 4-product Kaibel column. (Skogestad's method and Luyben's)

***Co-supervisor on all these projects: Maryam Ghardran and Ivar J. Halvorsen (SINTEF)***

## SIS-4: Control and optimal operation of Kaibel distillation columns

We have build an experimental column which is in operation. The obkective of the project is to design and test out advanced control strategies, for example MPC, both in simulation and in experiments.

***Co-spuervissor: Deeptanshu Dwivedi***

## SIS-5: Stabilization of two-phase flow in risers from reservoirs (anti-slug control) (in cooperation with Siemens)

These project are motivated problems with riser slugs in offshore fields in the North Sea. All projects are in cooperation with Siemens (Fredrik Dessen) and the multiphase group at the Department of Energy and Process Engineering (Prof. Ole Jørgen Nydal).

5.1: Control strategies for gaslift. First stabilization of standard gas lift is considered. Then the objective is to extend this to the case where also the topside valve is used as an MV. This will give two MVs which may be useful for extending the usuability.

***Co-supervisor: Esmaeil Jahanshahi (PhD student)***

5.2: Comparison and controllability analysis of alternative simple models for use for stabilizing control using topside measurements. (extension of project by Anette Helgesen)

1. Compare and analyze alternative simplified model of the process.
2. Controllability analysis
3. Use of advanced control based on topside measurements (Kalman filter, LQG etc.)
4. Implement on simulation (OLGA) and expreiment

***Co-supervisor: Esmaeil Jahanshahi (PhD student)***

5.3: Robust anti-slug control strategies. This will involve experimental work on three different rigs, and comparisons with models and dynamic simulation, with the objective to develop a robust anti-slug control scheme. For example, a hierarchy with flow control (or top pressure control), bottom pressure control and valve position control will be tested out.

***Co-supervisor: Esmaeil Jahanshahi (PhD student)***

## SIS-6: Dynamic simulation of alternative control strategies

The objective is to simulate and compare alternative base (regulatory) control structures on some case studies using dynamic simulation (Hysys/Unisim).

Links to descriptions of the software:

http://hpsweb.honeywell.com/Cultures/en-US/Products/ControlApplications/AdvancedControlOptimization/ProfitController/default.htm
http://hpsweb.honeywell.com/Cultures/en-US/Products/ControlApplications/Simulation/default.htm

***Co-supervsior: PhD student Ramprasad Yelchuru***

## SIS-7: Optimizing control of heat exchanger networks

The objective is to maximize the heat recovery during operation and identify possible self-optimizing variables. Possible applications include crude oil preheating networks and districting heating.

***Co-supervisor: PhD student Johannes Jäschke***

### SIS-8: A new method for soft sensing based on the nullspace method (self-optimizing control)

A new estimator based will compared with standard estimators (PLS, PCR) on several problems, ranging from standard challenge problems, as well as composition estimators for distillation columns, including Kaibel distillation columns.

***Co-supervisor: PhD student Johannes Jäschke and Maryam Ghardan***

### SIS-9: Controlled variables from operation data

By choosing a suitable control structure for a chemical process, it is possible to increase profits while keeping environmental and safety constraints in their specified limits.
Most conventional methods for determining a good control structure depend on the availability of a good process model. However, in many practical situations good models are difficult to obtain, because of the immense efforts required to develop and test a process model which is detailed enough to describe the process adequately, while easy to solve from a numerical point of view.

A different approach is to examine data from a given process, and to analyse it in order to find a control structure which gives good performance. This project involves studying how data from a given can be used to extract good control strategies.

***Co-supervisor: PhD student Johannes Jäschke***

### SIS-10: Toolbox for generation of nonlinear control models for semi-batch emulsion polymerization reactors

***The project is in cooperation with Cybernetica.***
***Reserved for Anette Hoel Helgesen***

## HP Professor Heinz A Preisig

### HP-1: Computer-aided modelling

We are building on a new tool expanding on three previous generations of modelling tools. The objective of this project is to provide a high-level modelling tool generating code for existing software tools, such as gProms or other simulation environments. The software implements a step-wise approach to modelling as it is being taught in the Control Course and the Systems Engineering Course. It builds on a graph representation of the processes, adds the "chemistry". A "theory" module provides the basic descriptions, like the balance equations and, where appropriate alternative transfer descriptions and kinetic laws, material descriptions and the like. The "theory" module is designed using a special tool, which implements a simple, tailored language.

The project could be any combination of the following:

- use the existing theory definition tool to include the main balances (mass, energy, momentum)
- explore the possibilities of using the tool for distributed systems.
- implement thermo component
- expand to include entropy

Recent publication: http://dx.doi.org/10.1016/j.compchemeng.2010.02.023

An excellent opportunity to learn more about modelling and if so desired, programming.

### HP-2: Control lab rejuvenation: Distillation

The department received 2.5 million NOK for the development of the felles lab and the control lab.
The control lab shall be updated and augmented with a couple of experiments. Initial plans have been developed. We invite to help thinking about possible, interesting processes and their realisation.

We have now rebuild the distillation columns but should further work on them. Objective is to move the heat exchangers down and make them more look and operate like its industrial counter parts. Besides other

issues I am thinking of implementing an original solution for on-line flow measurement and control of the reflux pump.

An excellent opportunity to learn about real-time programming, control and making experiments fool proof.

## HP-3: Control lab rejuvenation: A toy box

The department received 2.5 million NOK for the development of the felles lab and the control lab.

What is called the felles lab has a number of experiments we would like to look at and explore their potential to be tighter linked to a computing device, both on the measurement as well as on the control side.

Objective of the project is to improve the teaching value of the experiments by bringing them up to the current standard.

The idea is to use standard components on the measurement side, like pressure difference modules and circuits for temperature measurements using small scale, embedded-system based data acquisition and control devices.

## HP-4: Frequency Analysis of Distillation

Counter current processes show some very peculiar behaviours in the frequency domain. We have been analysing these behaviours in a couple of projects in the past: Ma, PhD on distributed models for tubular heat exchangers and the derivation of simple, but very accurate dynamic models. The findings have been verified in an experimental work done as a master thesis.
Recently we found a similar behaviour in distillation columns, which we would like to explore some more. Currently a project is ongoing looking into what looks like a simple linear counter current process, which has a structure similar to a distillation. This work should be continued towards a true distillation model. The work has potential to uncover a new methodology for identifying the internal dynamics in columns. It is thinkable that experimental work to that extent is added using the new-to-be-build columns in the felles lab.

## HP-5: Automatic Safety and Hazard Analysis

Safety and hazard analysis are done mostly in a systematic way, but based on mental models of the process. The most commonly used methodology is from the Sixties and was generated by ICI in England. It asks systematic questions to each stream in the plant, like what happens if there is no flow, what happens if there is much more flow, what happens if it flows in reverse direction, what happens if something else flows etc. The “what happens” is then filled in by experts, making up the basis for the analysis.
We would like to change this and use a model-based approach. Starting from a model of a continuous process, we have software that computes the possible things that may happen if the environment changes or faults occur.

Since we can do this computation, this method could be used to study if indeed something could possibly happen, which is precisely what a safety and hazard analysis does.

This type of analysis would give a systematic way of exploring the possible faults in a system, a subject of great interest to industry.

## HP-6: Process Identification using Wavelets

Wavelets are an exciting technology that allow the analysis of signals in time and frequency, in contrast to Fourier, that gives only frequency information. Wavelets are currently mostly used in signal processing as a data reduction processing. A common application is image processing. We are using the same technology for process identification. Essentially we can using wavelets to get derivatives to relatively high order on different level of resolution. This enables us to do identification on a multi-scale a technique matching the current development of multi-scale processes reaching from nano to industrial size equipment. I have also the vision that these technologies will enter the control field heavily in the future as these processes must be controlled across the scales. Thus some kind of plant-wide multi-scale process control.

We will introduce the student to multi-scale process modelling and wavelet methodologies.

### HP-7: Simple Thermo Server

The Process Systems Engineering group is heavily involved in process modelling particularly distillation. Distillation models and associated material models are used at a high frequency.

The project is aiming at implementing a server that provides:

- Interface requesting material information over the net
- Generic distillation simulation, freely configurable running on the server

The material model software is running and we are using it in a variety of ways. We thought it would be fun and very useful to build a little user interface that enables the interactive use of what the core can generate. This could then be put on-line in the form of a web page, for example.
We have a rather generic distillation column model that is quite generally parameterised, which could be augmented with an appropriate interface to make it usable on the web.

Such a system has been realised for Yara. A prototype sever exists and is currently operable for ammonia, nitric acid and urea production. The Matlab interface is already working and we are working on an interface to other computer languages such as Python.

An interesting task would be to use an interface to gProms
***Supervisosrs: Heinz A Preisig, Tore Haug-Warberg***

### HP-8: On time scaling in chemical processes

The Process Systems Engineering group is heavily involved in process modelling. The objective is to generate a very general framework in which models for the process industry can be generated quickly and rapidly.
Making time-scale assumptions is done very frequently in the modelling process. Mostly it is not really done explicitly, but just kind of happens. Examples are decision on how to model a heat transfer, for example using an overall heat transfer model is making a time-scale assumption about the distributed transfer system to be of negligible capacity. Similar assumptions appear all over the place and we would like to put this problem into a more systematic framework.

The problem of getting measures for the relative dynamic of parallel fundamental transfer process is a common problem in chemical engineering. Probably best known are the “modules” such as the Thiele modules and dimensionless numbers. The derivation of such modules is very frequently based on “pseudo steady-state” assumptions, which in mathematical terms is a standard singular perturbation.

The project should look into the literature and analyse the mechanism behind the derivation of the different modules and the like with the aim of deriving a generic understanding behind these measures. In the next stage we want to know if such measures are useful in deciding if or if not the underlying pseudo steady-state assumption can be made or not and if possible on how wrong one is if one does make the assumption dependent on the dynamics.

## *TH-W: FørsteamanuensisTore Haug-Warberg*

### TH-W-1: Multi-phase equilibrium calculations

**Full title:** An algorithm for multi-phase equilibrium calculations using generic thermodynamic information only.

**Background:** The generic thermodynamic equilibrium calculation is a cornerstone in all chemical engineering calculations involving the reaction and separation of multicomponent systems. A major breakthrough in this field of science was done around 1980, and till this day several hundred different algorithms have been published worldwide in the international engineering journals. However, so far no algorithm has proved superiority in every respect with respect to robustness, flexibility and speed. It is

therefore of great interest, both theoretically and practically, to examine the state of art in this field and to come up with a suggestion on how to solve the generic multiphase problem. Generic in this context means that the constraint situation (constant T, constant p, constant V, etc) shall be a run-time calculation attribute. This stands in stark contrast to the situation where several different algorithms are built to handle each of constraints. The latter approach is maybe the most efficient with respect to computation time, but it renders the user with a very heavy burden of maintenance problems. It is also important that the robustness is parameterized such that it is possible to steer the expected computation time from low (less robust results) to high (more robust results). The initialization of any equilibrium calculation is usually a big problem and it is tempting to use all sorts of physical information for this purpose (like e.g. the critical point and the boiling curve). This reduces the flexibility of the algorithm, however, and the initialization should therefore be based on generic information only (chemical potentials typically).

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**Goal:** 1) Conduct a review on the state-of-art of phase equilibrium algorithms. 2) Implement a multiphase equilibrium prototype in Matlab showing the features mentioned above for the T,V constraint case. 3) Broaden the base case by considering other constraints like T,p and S,V and H,p etc. 4) The algorithm shall be tested on practical (experimental) problems and theoretically hard problems from the literature. An alternative to task 3) is to re-implement the Matlab prototype in C/Lua or another open-source alternative to Matlab (which is crucial for later re-use of the code).

**Prior knowledge and experience:** The student must show an interest in computer programming and numerical mathematics, and must have a fair background in physical chemistry and thermodynamics.
***Supervisor (NTNU): Ass. prof. Tore Haug-Warberg***
***Co-supervisor (SINTEF): N.N. (not clarified, but I would expect Olaf Trygve Berglihn, Bjørn Tore Løvfall, Magne Lysberg or John Morud to be interested in this work)***
***Reserved: Silje Kreken Almeland***

## NS-B: Førsteamanuensis Nadi Skjøndal-Bar

### NS-B-1: Systems Biology - Modelling and analysis of the process of initiation control in protein synthesis

Systems biology is a fascinating field that aims at system-level understanding of biological systems. What does it mean to understand at ”system level”? Unlike molecular biology which focus on molecules, such as sequence of nucleotide acids and proteins, systems biology focus on systems that are composed of molecular components. Although systems are composed of matters, the essence of system lies in dynamics and it cannot be described merely by enumerating components of the system. Within this context, (1) understanding of structure of the system, such as gene regulatory and biochemical networks, as well as physical structures, (2) understanding of dynamics of the system as well as construction of theory/model with powerful prediction capability and (3) understanding of control methods of the system, are key milestones to judge how much we understand the system. There are numbers of exciting and profound issues that are actively investigated, such as robustness of biological systems, network structures and dynamics, and applications to drug discovery.
It was found in the last decade that gene expression is mainly effected by the initiation process. Eukaryotic initiation factors (eIF-) 2 are molecules exist in almost every cell of our body. They were found to regulate gene expression, by enabling a ribosome structure to bind to a pre-initiation complex. This process is complex and involves many different regulating components. A simplified model of the eIF-2 regulation process was developed using a non-linear state space framework (see Bar and Morris, 2007). Simulations and analysis of the reduced model led to several conclusions about the effect of a few principle factors in the eIF-2 initiation process, consistent with recent experiments in yeasts.
The aim of the Project includes: (1) a background study of the eIF-2 regulation process (2) Exploration of robustness of the model to noise (disturbances) and (3) sensitivity analysis of the model. Pre-knowledge in biology, genetics, and molecular biology is an advantage, but is not essential for the success of the Diplom. The candidate can easily establish a career in Systems

Biology as modeler, researcher and systems engineer both in the industry (for instance in medical companies) and particularly in the academy (PhD programs all over the world).
Further details about the project thesis can be acquired at 735-94124 or email nadi.bar@ntnu.no
Further reading:
Systems biology:
H. Kitano, Systems Biology: a brief overview, Science, 295:1662-1664, 2002
H. Kitano, Computational Systems Biology, Nature, 420:206-210, 2002
Control of Protein Expression:
N. Skjøndal-Bar and D. Morris: Dynamic model of the process of protein synthesis in Eukaryotic cells, B. math.Bio, 69:361-393, 2007
1***Supervisor: Nadi Skjøndal-Bar***

## NS-B-2: Systems Biology - Gastrin modelling Project

Gastrin is a hormone mainly produced in response to food and is under negative feedback regulation by gastric acid. Gastrin is suggested to be involved in autocrine growth regulation in gastrointestinal and stem cell derived tumours, causing lethel cancer.
NTNU has an ongoing Gastrin project, led by Dr. Astrid Lægreid, at St. Olavs Hospital. The project consists of 6-7 scientists and about 6 Phd Students. The prosess to understand the gastrin network is complicated due to the large number of components (genes, proteins), and therefore a system level of understanding is required. Mathematical models are excellent tools to facilitate understanding of complex systems as the gastrin network, and are used by our group at several levels.
The main purpose of the project: Use (simulate, analyse) an already existing mathematical model (dynamical) to explains existing observations in the gastrin network, and develop new hypotheses emerging from the dynamical model. This incudes the use of Network Component Analysis method (NCA) the extract the data needed for the dynamical model.
The main supervisor is Nadi Skjøndal Bar, expert in modelling and analysis of biological systems, and is assisted by 2 Phd candidates which will co-supervise the student to provide the Master student full support.
Further information call 94124 or email nadi.bar@ntnu.no
**Supervisor: Nadi Skjøndal-Bar**

# Miljø- og reaktorteknologi/Environmental Engineering and Reactor Technology Group

***Reaktor Technology***

## *HAJ Professor Hugo Atle Jakobsen*

### HAJ-1: Numerical investigation of integrated reactor-separator designs for pre-combustion with $CO_2$ Capture.

Based on models of different complexity for describing fluidized bed and fixed bed reactor process performance various reactor designs will be evaluated for the steam methane process with $CO_2$ capture. A superior purpose with this investigation is to decide which of these two reactor types is best suited for the given process.

In this work we intend to simulate the whole process cycle considering the reformer reactions, adsorption of $CO_2$ and desorption of $CO_2$ from the adsorbents. To optimize the reactor performance with $CO_2$ capture, we may consider the possibility to reduce the operating temperature, reduce the reactor volume, lower pressure, intencify heat integration and to reduce emissions fluxes compared to the conventional steam methane reformer process. The first part of the work consists in deriving suitable models for the different reactor types. Then, the models should be implemented in matlab and solved with a suitable numerical method.

*It is possible to split the project into two parts so that one student may study the process operated within fixed bed reactors and a second student investigate the process operated within fluidized bed reactors.*
***Supervisor: Hugo A. Jakobsen***

### HAJ-2: Numerical analysis of multicomponent mass diffusion in catalyst pellets for combustion with and without $CO_2$ capture.

A consistent model for multicomponent mass diffusion is derived and we want to perform model validation. Tradidionally the Maxwell-Stefan model has been formulated in terms of mol-fluxes and not mass-fluxes. This approach is limiting the application of the Maxwell-Stefan formulation because the heat and momentum balances are normally formulated in terms of mass averaged velocities and not molar averaged velocities. We intend to prove that the novel mass based formulation is consistent with the conventional molebased formuklation.

For this purpose we may use the catalyst pellets for steam metan reforming (SMR) and the pellets for sorption enhanced steam metan reforming as test examples. Furthermore, we need to evaluate whether the convective terms in the model can be neglected or not to validate a common assumption in reactor modeling.

These models will be implemented in Matlab and solved by ortogonal collocation.
***Supervisors: Hugo A. Jakobsen and Magne Hillestad***

### HAJ-3: Numerical investigation of the chemical looping combustion/reforming (CLC/CLR) processes.

Based on models of different complexity for describing the fluidized bed reactor processes performance various reactor designs will be evaluated for the CLC and CLR processes.

In this work we intend to outline the possible reactor designs and to model and simulate a few of the possible reactors for these processes. To optimize the reactor performance with $CO_2$ capture, we may consider the possibility to reduce the operating temperature, reduce the reactor volume, lower pressure,

intencify heat integration and to reduce emissions fluxes compared to the conventional processes. The first part of the work consists in a literature review to find physical data, transport coefficients, reaction equilibrium and kinetics models, and as a second part of the work suitable models for the different reactor types must be formulated. Then, finally, a few (at least one) models should be implemented in matlab and solved with a suitable numerical method.

*It is possible to split the project into two parts so that one student may study the CLC process and a second student investigate the CLR process operated within fluidized bed reactors.*
***Supervisors: Hugo A. Jakobsen, Magne Hillestad and NN from Catalysis group***

## HS: Professor Hallvard F. Svendsen

### *Relatet to $CO_2$-capture:*

#### HS-1: Characterization and modeling of L/L systems

The purpose of the projects is to map various $CO_2$ – amine systems regarding VLE for $CO_2$, VLE in unloaded and loaded systems and the two phase region as function of $CO_2$ loading and temperature. These data will then form the basis for a consistent equilibrium model.
***Faglærer/Veiledere: Hallvard Svendsen/Ardi Hartono/Inna Kim***
***The project is reserved for Christian Jens***

#### HS-2: VLE in single and two-liquid phase systems

The purpose of the projects is to map various $CO_2$ – amine systems regarding VLE for $CO_2$, VLE in unloaded and loaded systems and the two phase region as function of $CO_2$ loading and temperature. These data will then form the basis for a consistent equilibrium model. The system will be different from project 1 and the apparatuses as well.
***Faglærer/Veiledere: Hallvard Svendsen/Shahla Gondal/Ardi Hartono***
***The project is reserved for Syed Zaidy***

#### HS-3: VLE and solubility in absorbent systems

The aim is to produce consistent set of data for many absorbent and $CO_2$ concentrations, and for the temperatures 25, 40, 60, 80, 100, and 120$^oC$. The systems to be investigated are amine and amino acid systems. In addition the $CO_2$ solubility in these systems will be determined. The data will form the basis for a consistent equilibrium model.
***Faglærer/Veiledere: Hallvard Svendsen/Shahla Gondal/Ardi Hartono***
***The project is reserved for Fahad Saleem***

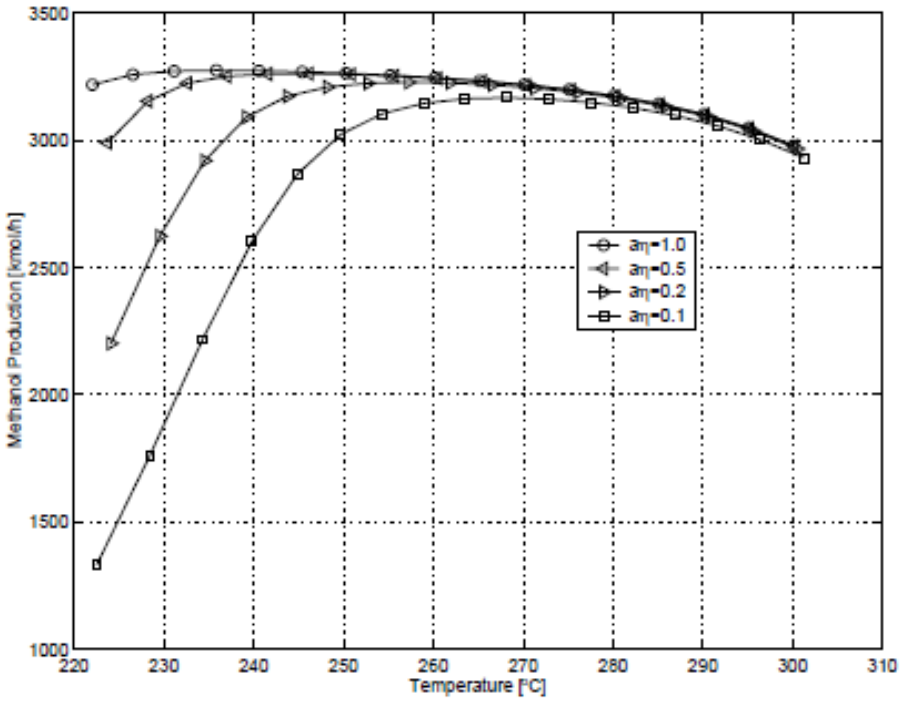
#### HS-4: $CO_2$ absorption: Calorimetric measurements.

One of the most important properties of new absorbent systems for $CO_2$ capture, are their thermal behaviour. We need to know the heat of reaction as function of temperature and $CO_2$ content. Some system, in particular 2nd and 3rd generation solvents may undergo phase change. This we also need to understand and characterize fully. The measurements will take place in a calorimeter and involve liquid phase analysis. The thermal data will be analyzed using a rigorous thermodynamic model, either the extended UNIQUAC model or the eNRTL model.
***Faglærer/Veileder: Hallvard Svendsen/Anastasia Trollebø***
The project is open

## MH: Professor Magne Hillestad

## MH-1: The effect of operational parameters in a methanol plant

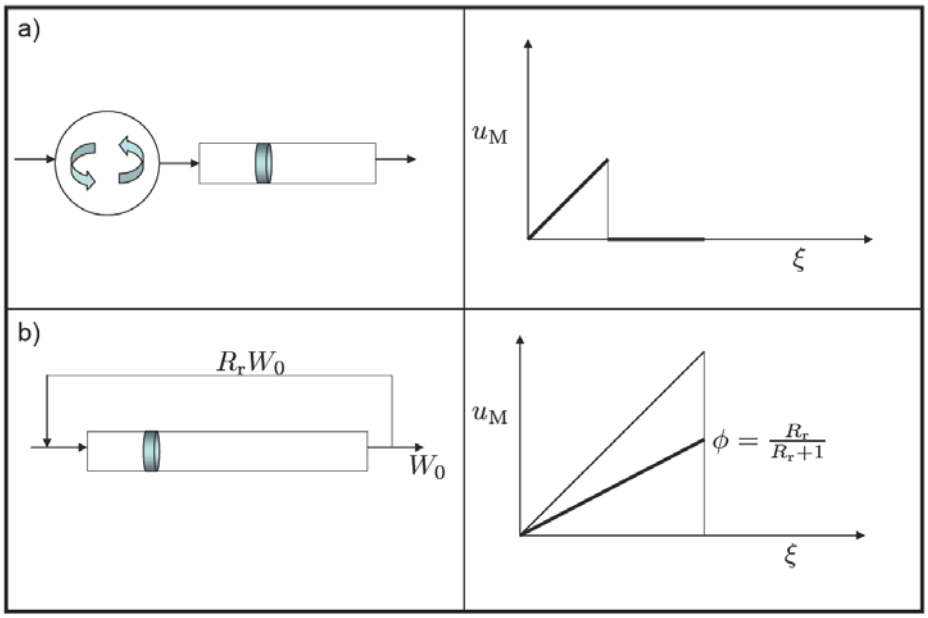
Statoil's methanol plant at Tjeldbergodden converts natural gas to methanol. The plant consists of an air-separation-unit (ASU), syngas production, methanol synthesis and raw methanol distillation. This project will focus on the methanol synthesis loop.




There are a number of operational parameters that is of interest to look at, such as recycle ratio, syngas composition (makeup gas), temperature and pressure. The effect of these parameters will change with the catalyst activity. It is of interest to study the effect of different parameters at different catalyst activities (combination of activity and effectiveness factor). The synthesis loop can be modelled in Hysys, UniSim or Matlab with a published kinetic model.
Focus will be on new design of the methanol synthesis.
***Supervisor: Magne Hillestad***
***Reserved: Kristian Bøhn***

## MH-2: Systematic Staging in Chemical Reactor Design

For economical and environmental reasons, it is of paramount importance to develop process technologies with improved material and energy efficiencies. The input factors such as raw material and energy should be utilized to produce valuable products, with the use of least possible equipment volumes and areas. A simple criterion is space-time-yield, but other criteria that include energy efficiency should also be considered.




The core of a chemical plant is the reactor. A method for systematic staging of chemical reactors will be further developed and applied on a published kinetic model. Reactants pass through a series of functions or basic operations to form the desired products. The basic operations are represented by design functions on the volume path. The design functions are fluid mixing (dispersion), distribution of extra feed points, distribution of heat transfer area and coolant temperature, catalyst dilution distribution and more. The conceptual reactor design problem is solved as an optimal control problem. Parameterization of the design functions and the state variables are applied. The realization is a staged process string of multifunctional units. A kinetic model of the gas phase methanol synthesis is used as an example. By applying the method on the model, a staged reactor design with less heat transfer area and higher production is possible.

The method is to be applied on a known system where the kinetics and other phenomena are described. The model will be programmed in Matlab or Python.
***Supervisor: Magne Hillestad***

## MH-3: Dynamic modelling and simulation of a CO2 capture plant

We will focus on dynamic modelling of a post-combustion capture plant based on an amine solution. The motivation is to evaluate the process design and operational philosophy of the plant. By dynamic simulation we will analyse how the plant is able to handle large load changes, startup and shutdown procedures, flue gas composition changes, etc. Based on the simulations the design and operational procedures, including process control are to be evaluated and if necessary improved. The model of the absorber may be modeled as plug flow both for gas and liquid.
***Co-advisor: Hanne Kvamsdal, Sintef***

## MH-4: Modelling and optimization of a Gas-to-Liquid plant

A GTL plant consists of syngas production, Fischer-Tropsch (FT) synthesis, and FT products upgrading. The first stage is production of syngas form different feedstocks (natural gas, coal and biomass). Different technologies have been developed for syngas production unit such as: Adiabatic Pre-Reforming, Steam Methane Reforming (SMR), Auto Thermal Reforming (ATR), gas-heated reforming and series or parallel combinations thereof. In the FT unit the syngas is converted to liquid fuels on an iron or cobolt catalysts. There exist different reactor configurations for FT units. We have simulated syngas and FT units using Unisim Process Simulator (Xu and Froment kinetics model (1989) for Syngas unit and Satterfield kinetics model (1990) for Co catalysts).

After simulation of these units, we will introduce an objective function and then find the optimal values of process conditions and equipment sizes.

The optimization phase deals with:

- Evaluating the possibility of production of Syngas from different feedstocks,
- Applying available technologies and arrangements for Syngas and FT units,
- Possibility of producing methanol or ammonia from Syngas rather than FT products in one site and determine the optimum production rates of each one.
- Heat integration of streams.

***Co-advisor: Ahmad Rafiee***

## MH-5: Energy considerations around an amine $CO_2$ capture plant

Adding a $CO_2$ capture plant to a power plant will introduce a penalty up to 30%. A post combustion $CO_2$ capture plant will consist of an absorption column, a stripper, heat exchangers, a blower, pumps, $CO_2$ compression. The most energy requirement is the steam for stripper.
The aim of this project is to find the suitable solvent and operating condition and best configuration to reduce the energy consumption for a post combustion capturing plant. This project has three main tasks. The tasks are as follows:

- Solvent investigation and comparison for $CO_2$ capture
- The irreversibility in capturing plant and the effect of it on energy consumption
- Compare different alternative configuration for capture plant

In addition to analytical models, the capturer plant can be modelled in UniSim, Hysys or Aspen plus.
***Co-advisors: Mehdi Karimi and Karl Anders Hoff (SINTEF)***

## MH-6: Fouling monitoring of Condenser at Snøhvit

The main condenser at Snøhvit, where ethane and propane are liquified, need to be monitored with respect to fouling. The following activities are anticipated:

- Literature survey
- Modelling of phase change (dewpoint calculation)
- Model the exchanger with the front of phase change and temperature profile along the condenser.
- Tuning of model against plant measurements.
- Calculate/estimate the fouling based on historical data.

***Co.advisor: Arne Olav Fredheim, Statoil***
***Reserved Rebecca Williams***

## MH-7: Energy Utilization in EDC Cracking

Vinyl Chloride (Chloroethene, VCM) is mainly used for the production of the commodity plastic Polyvinyl Chloride (PVC). The main commercial route to VCM today is balanced, ethylene based production, see block diagram. INEOS ChlorVinyls is one of the major chlor-alkali producers in Europe, a global leader in chlorine derivatives and Europe's largest PVC manufacturer. INEOS ChlorVinyls operates four VCM plants in Europe; Rafnes in Norway, Runcorn in Great Britain, Stenungsund in Sweden and Wilhelmshaven in Germany.

The largest single energy consumer in the balanced process is the EDC cracking section, in which 1,2-Dichloroethane (EDC) is thermally dehydrochlorinated to VCM. This reaction is highly endothermic ($\Delta H$= 71 kJ/mol) and the heat of reaction is supplied by combustion of fuels such as natural gas, hydrogen or oil. An Aspen Plus model is available for the energy and mass balance of the EDC cracking section. A project using this model as the basis for investigating the possibilities of increasing the energy performance of the cracking section is proposed. Of particular interest is an exergy analysis of the EDC cracking section.

The project may include:

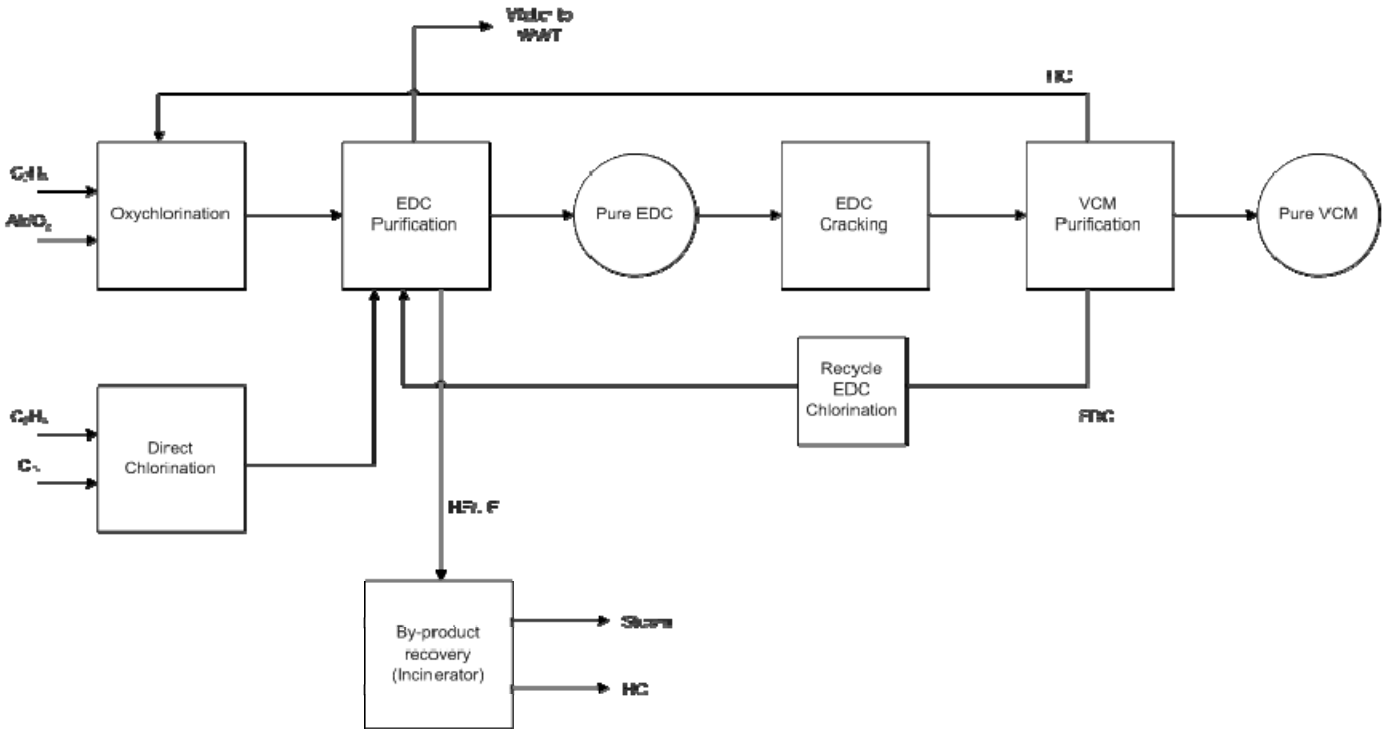
1. Develop methodology for performing exergy analysis using Aspen Plus model

2. Perform exergy analysis for different operating conditions
3. Perform pinch analysis of the EDC cracking section

Points 1 and 2 are prioritized

The work will be conducted in cooperation with INEOS ChlorVinyls Technology & Production Support in Porsgrunn.

This project will serve as a natural basis for continuance into a diploma work where the energy efficiency of all four sites is compared.




***Co-advisor: Ineos ved Torbjørn Herder Kaggerud***
***Reserved: Stine Karlsen***

## MH-8: Part load performance of power plant with CO2 capture

In the campaign of mitigating CO2 emissions we move towards a more complex energy system where the dependence on renewables and other carbon neutral energy sources will lead to larger variations in electricity demand from power plants. Also variations in energy prices will require a higher degree of flexible operation. Several parameters in the power plant are affected during part load operation, such as flue gas and steam flow rates, flue gas composition, temperature and pressure levels. To get an understanding of how these variations occur and what challenges they inflict is of value. Vital parts of the process should be identified, e.g. steam extraction pressure from the power plant.
***Co-advisor: Paul Ystad***

## MH-9: Dehydration and compression of contaminated $CO_2$-rich gas

A large part of the worlds remaining natural gas reserves contains considerable amounts of carbon dioxide ($CO_2$) and hydrogen sulphide (H2S). Both these components need to be removed to low levels export or use it for fuel. The European gas quality specification for maximum acid gas content is 2.5vol% $CO_2$ and 5 mg/m3 H2S [1].

In order to reduce $CO_2$-emissions, the $CO_2$ that is removed from the natural gas can be compressed and stored in a suited reservoir. The $CO_2$-rich off gas from an acid gas removal unit may contain contaminants such as nitrogen and hydrocarbons. This affects the phase behaviour of the $CO_2$-rich off-gas. If the impurities are not accounted for during design of the $CO_2$ dehydration and compression system, operational

problems like vibrations loss and cavitations in pumps may occur. The capacity of the system will also be affected. The exit pressure must be increased in order to produce a fluid that can be injected. Finally, there is an unwanted loss of hydrocarbons with the injected $CO_2$.

The topics of the master thesis will be:

- Litterature review on
  - Collection of literature equilibrium data for the system $CO_2$-$H_2O$-$CH_4$-$N_2$
  - State-of-the-art system designs for $CO_2$ dehydration and compression
- Compare equilibrium data for the $CO_2$-$H_2O$-$CH_4$-$N_2$-system with the predictions in Pro/II or HYSYS.
- Simulation of a state-of-the-art $CO_2$ dehydration and compression systems in Pro/II or HYSYS.
- Evaluate the effect of impurities on the dehydration and compression designs
  - Type of impurity
  - Concentrations of impurities (up to 5 mol%)
- Evaluate alternative ways to handle impurities in the $CO_2$-rich gas including
  - Design margins required in standard designs
  - Modifications of standard designs

1. CBP 2005-001/02 Gas Quality Harmonisation, (http://www.easee-gas.org)

***Co-advisor: Eivind Johannessen, Statoil***
***Reserved Vidar Graff.***

## *MSc-project proposals from the Membrane Research Group*

## *M-BH Professor May-Britt Hägg*

### M-BH-1: The effect of high pressure and vacuum on FSC (fixed-site-carrier) membrane performance for $CO_2$ separation for flue gas

The application of membrane for $CO_2$ capture is getting more attention because of the simplicity, lower energy cost and environmental friendliness compared to the potentially hazardous solvent (alkanolamines) absorption method.

An excellent FSC membrane for $CO_2$ capture has been under active development in MEMFO group (IKP, NTNU) and is going to be tested and estimated in pilot scale and industrial scale soon.

But for further scale-up to pilot and industrial scale application, even wider range study on process parameters is required to simulate and optimize process design and to meet the industrial requirements.

This wider range study has been partly performed during 2010 fall project which focused on expanding the span of data and knowledge by applying higher pressure and vacuum. The results show clearly that further study and continuation of this project are inevitable.

1. From the 2010 fall project, where a new vacuum pump was installed in the lab-scale set-up and tested, it was found out that realization of vacuum on permeate side is complicated and challenging more than expected due to instability of the system (partly by vacuum pump operation), drying of the permeate side of the membrane and/or more water permeation through membrane depending on the level of vacuum pressure. So this study will be continued.

2. Meanwhile the installation/operation of the pilot scale membrane test set-up could not be fully completed during 2010 fall semester, the operation of the pilot set-up is expected to be normalized in the next semester. So the performance test of the FSC-membrane in a large scale module in a pilot scale set-up and the data/results will be a quite interesting & very important task for the 2011 spring semester, too.

3. The change of membrane performance after exposure to some industrial contaminants, especially $NO_2$, will be investigated while seeking a possibility of enhancing the performance by some other ways.

4. All the experiments will be accompanied with suitable characterizations of the membranes using NMR, amine titration, SEM, swelling test, etc.

***Co-supervisor: Dr. Taek-Joong Kim***
***The project is reserved for Anna Elise Leithe***

## M-BH-2: Optimization of the CNTs reinforced PVAm/PVA blend membranes

This master thesis will focus on the optimization of the carbon nanotubes (CNTs) reinforced polyvinylamine/polyvinylalcohol (PVAm/PVA) blend membrane for high pressure gas separation applications, such as natural gas sweetening process. CNTs are considered as the nano-fillers in making the PVAm/PVA blend based nanocomposite membranes. The functions of the CNTs in this membrane include the reinforcement of the membrane mechanical properties and the improvement of the membrane swelling capacity (and hence $CO_2$ separation efficiency) at high pressures due to the nano spacer effect of the CNTs.

The tasks of this thesis work can be specified as follows:

1. Selection and modification of commercially available, water dispersible CNTs

2. Optimization of the dispersion of selected CNTs in blend solutions The CNT loading, CNTs dispersion protocol and the concentrations of casting solution will be optimized, possibly with an orthogonal experimental design.

3. Permeation test of the CNT-blend membranes

4. Characterizations of the CNT-blend membranes

Further characterizations of the CNTs-blend membranes will be carried out to quantify the improved properties, including mechanical strength, SEM, FTIR, XRD, sorption of gases at high pressures.

With results from above listed work, this project may contribute significantly to the commercialization of the FSC membrane in the natural gas sweetening process and further more, to the promotion of the green and energy saving membrane approach in $CO_2$ capture solutions. Creativity in this project is highly appreciated.

***Co-supervisor: Dr. Liyuan Deng***
***(Not reserved – competence from Basic Membrane Course needed)***

## M-BH-3: Investigation of new polymeric membranes with controlled architecture for $CO_2$ capture

The project represents collaboration NTNU (IKP, Memfo group) with University of Montpellier, Institut Européen des Membranes Adaptive, Supramolecular Nanosystems Group. The focus of the project consists on screening of new materials as new membrane materials for $CO_2$ capture.
The first part of the project represents a literature study exploring the potential of different co-polymer membranes consisting of different polymers such as poly(dimethylsiloxane), tri-aldehide, tri-amine, histamine, etc obtained by poly condensation (see Fig. 1 as an example) for gas separation with focus on $CO_2$ capture from flue gas and natural gas sweetening.

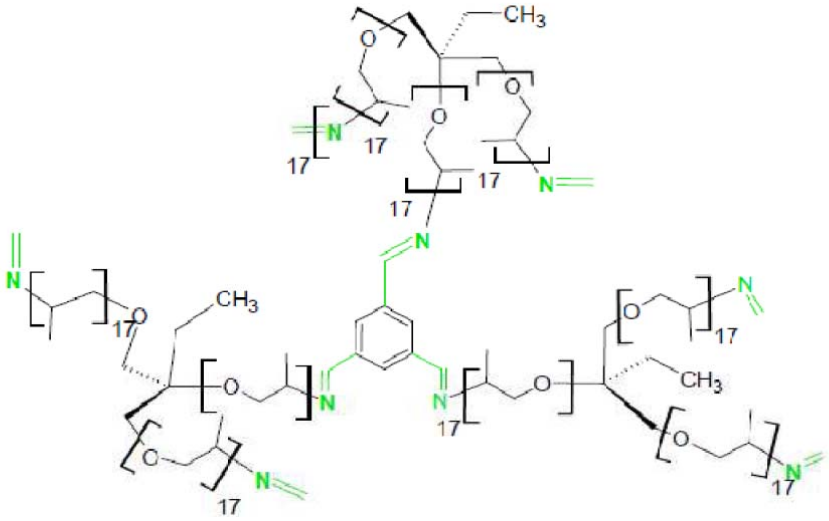


Fig. 1 Triamine Ethyl Glycerol

The second part of the project consists of experimental study. The membranes material, different blend ratios, will be investigated by IR, DSC and gas sorption.
The membranes will be investigated by gas permeation. The gas permeation experiments will be performed under different controlled parameters: pressure, gas composition, temperature and humidity.
***Co-supervisor: Dr. Marius Sandru***
***Reserved for Mohammad Mashukur Rahman***

## M-BH-4: Preparation of high $CO_2$ permeance and selectivity PVAm/PSf composite hollow fibers

Processing large volume of gases from industrial sources requires a large membrane area with a minimal foot print. Hollow fibre membrane geometry represents optimum solution due to the high ratio of membrane area per volume.
Polysulfone hollow fibers presenting high $CO_2$ permeance were produced and investigated in a previous master project (student Ragne M.L. Helberg) see Fig.1.
The assignment requires a literature study and practical experiments. The literature study will be focused on finding suitable polymers for protective coating such as chitosan, polyvinyl alcohol, PDMS, and other suitable materials. The literature study will investigate different coating techniques for thin films such as dip coating.
The laboratory work will consist in PSf hollow fiber membrane coating with a selective layer of PVAm followed by a protective coating. The membranes will be investigated by scanning electron microscopy (SEM), gas permeation (before and after coating).

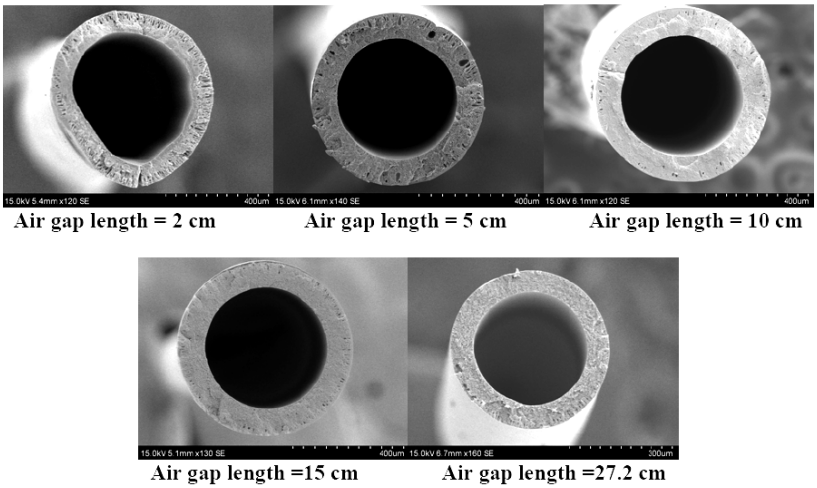



Fig. 1 PSf hollow fibers produced at NTNU

The project will be focused on coating procedure optimization for hollow fibre polymeric support with a $CO_2$ selective and defect free polymeric layer. A special focus of research will be on polymer, solvent and coating technique choice. Different parameters will be optimised to obtain highly permeable protective coatings and highly selective coatings: polymeric solution concentration, choice of solvent, coating procedure and drying protocol. The coated hollow fibres will be packed in modules and membrane separation properties will be tested for different gas mixtures such as $CO_2/N_2$, $CO_2/CH_4$.

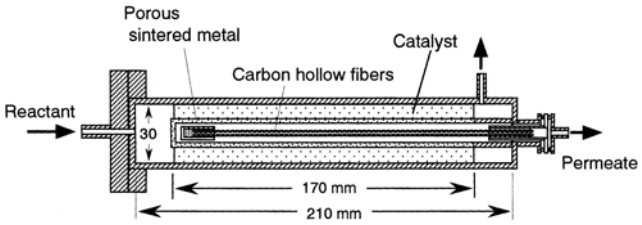
Module design for gas permeation will be optimized for different pressures, gas mixtures and gas flow patterns. The packing density of hollow fibers, the sealing procedure, the operating conditions (sweep or vacuum in the permeate side) and the intrinsic module design represents key factors for an efficient gas separation.

***Co-supervisor: Dr. Marius Sandru***

***(Not resereved – competence on Basic Membrane Technology needed)***

## M-BH-5: Carbon membrane reactor

The two most important steps in a chemical process are usually the chemical reactor and the separation of the product stream. Both the process economics and the efficient use of natural resources could be improved by the combination of these two processes into a single unit operation, leading to potential savings in energy and reactant consumption and reduced by-product formation. The application of membranes in reaction engineering has steadily been more and more promoted. Although both inorganic and polymeric membranes can be incorporated with reactors, there are a limited number of reactor applications for polymeric membranes because of their limitations with respect to high temperatures. There is, however, a growing interest in inorganic catalytic membrane reactors since it may offer more opportunities over a wider range of operating temperatures. One of the latest interesting development with respect to inorganic membrane reactors is the carbon membrane reactor (see figure). Very few references are found on carbon molecular sieve (CMS) membrane reactors, although these materials exhibit high performance with respect to both permeability and selectivity, they are relatively inexpensive, and may be applied at high temperatures. One reason for the few references may be that relatively few research groups are working on funtionalization of the hollow precursor fibres needed for carbonization to CMS membranes. According to our judgement, the *functionalized* CMS fibres show a high potential for application in CMS membrane reactors for high temperature catalytic reactions.




In the current project we will investigate the possibility of coating a ceramic tube with a polymer, and then carbonize it according to a given protocol which will be suitable for separation of CO2 – H2 by allowing H2 to permeate and $CO_2$ being retained. Functionalization of the carbon membranes will also be tried. The project will focus on development of a good separation membrane, suitable for being used as a membrane reactor in the next round. The effect of high temperatures (→ 450°C) on the separation will be investigated.

***Co-supervisor: Dr. Qiang Yu***

***Reserved for Juan B. Freire Lopez***

## M-BH-6: Osmotic Membrane

Inflow control device is a technology for controlling the inflow of gas, oil and water from the reservoir to the wells. Inflow control devices have become increasingly important as measures of improving production and reservoir management. The focus of this study is autonomous inflow control technology for choking of water in gas-condensate wells. The technology uses the principle of osmosis to actuate a valve and is termed; Osmotic membrane pressure actuator (OMPA). The technology is proved to work in a low pressure and low temperature environment using fresh water, crude oils and different osmotic agents. FO membranes (cellulose acetate and polyimide) were already tested at Telemark University College and

Statoil, but further investigations are needed. The tested membranes do not meet the requirements of high temperature conditions in the well although theoretically the polyimide material can withstand up to 300°C. A preliminary screening of membranes executed in 2010 show that no suitable membrane with the properties to with stand high temperatures exist. It is therefore of interest to investigate other possibilities in the current project.
A suggested scope of work will be:

1. ***A literature study*** on materials that can withstand temperatures up to 200°C to be used for membrane development will be given together with a strategy on how to prepare the membrane.
2. ***Membrane specifications*** will be identified using the well conditions from a specific field. An overview of eventual challenges as e.g. fouling that must be solved to satisfy the functional requirements will be given along with recommendations on how this can be done.
3. ***Laboratory Testing of membranes*** to measure the properties of the forward osmosis membranes, starting with testing them in RO mode. The pore size, water flux, retention will be measured by standard characterization techniques.
4. ***Initial preparation/synthesis of new membranes*** that can withstand the conditions in a reservoir

The membrane should be able to provide reversibility, acceptable resistance against fouling, have a long lifetime and high integrity.

***Supervisor: May-Britt Hägg in collaboration with Statoil***
***Co-supervisor: to be appointed later***
***Reserved for Jonathan Ashley Greene***

### M-BH-7: Membrane Contactor

Membrane contactors are an alternative technology for removal of $CO_2$ from natural gas or flue gas, and is in reality a combination of membrane separation and removal by plain absorption. The Memfo group is partner in a project with Sintef and several Oil & Gas companies where this technology is to be investigated. The MSc-project offered here, will be part of this project. Investigation on alternative membrane materials to be used; alternative solvents, calculations of mass transfer coefficients documented by experimental results will be important. Details in the MSc-project will be elaborated on before start-up as it also depends on activities in a PhD-project in the same research project.
***Co-supervisors: Dr. Taek-Joong Kim; PhD-student Karen Nesssler Seglem***
***Reserved for Mohammad Saeed***

### M-BH-8: Membrane process simulations

The membrane separation to be investigated, is a selected process from process industry; for instance cement idnustry, $CO_2$ removal from flue gas. The flue gas from this application has a somewhat different composition than flue gas from power plants, and will have other considerations with respect to environmental issues and process conditions. The volumes to be handled will also be somewhat lower. For the simulations, an in-house program for membrane separation (Chembrain) which is interfaced to Hysys, will be used. Economical calculations for the process should also be performed. In the MSc-thesis it should also be considered the alternatives for sequestration and transport from a selected cement plant. Details on the work to be performed in the MSc-thesis will be more detailed out before start-up of the work.
***Co-supervisor: Dr. Arshad Hussain***
***Reserved for Ola Kjølberg Haglund***

## *Crystallization*

## *J-PA: Førsteamanuensis Jens-Petter Andreassen*

**J-PA-1: Investigations of pre-treatment in MEG-regeneration by precipitation.**

(In co-operation with Aker Solutions)

Aker Process System (APS) is a business unit within Aker Solutions. We strive to be a leading global supplier of selected process systems based on proprietary technology and APS is one of the world main suppliers of technology for hydrate inhibition in gas processing.

During transportation of multiphase from (hydrocarbon gas/condensate/water) Mono Ethylene Glycol (MEG) is used as an"antifreeze" agent preventing formation of natural gas hydrates in the pipelines. In addition to condensed water, water from the reservoir is also produced with the gas either initially or in later life-time of the wells. This water (formation water) contains salts (for example $Na^+$, $K^+$, $Ca^{2+}$, $Mg^{2+}$, $Fe^{2+}$, $Cl^-$) which can form scale/solids in the regeneration process. The glycol is regenerated in a MEG regeneration unit which removes water and salts enabling re-injection into the process as fresh inhibitor. The amount of salts in the formation water will determine the risk and amount of precipitated solids in the MEG and the variation in temperature and pressure along the process initiates different degree of precipitation. The potential amount of precipitated solids can vary from some kilos per day to several tons dependent on the composition of the formation water.

The pre-treatment is an important part of the MEG regeneration process in where the divalent cat-ions are separated from the MEG by increase of supersaturation to aid precipitation as particles, followed by liquid solid separation. Solids from the divalent cat-ions are small crystals which may be difficult or time consuming to separate from the solution. To promote the precipitation alkaline chemicals are added. The mixing of the alkaline chemicals into the process stream can change the nucleation rate and the crystal size distribution, and thus different methods for mixing might improve the control of the precipitation and optimize the process. The preferred mixing method should give the larger crystals which are assumed to separate more easily. The crystal size can also be increased by flocculation and aggregation as an effect of addition of additives. Both mixing and addition of additives can be investigated in this project.

The objective of the assignment is to improve the precipitation in the pre-treatment and the following separation process. The approach will be to test different procedures for mixing of the alkaline chemical into the solution (location, temperature at mixing point, effect of agitation etc.), and investigate how sensitive different mixing variations is to the size and shape of the precipitated product. It will also be necessary to test the sensitivity of the strength of the alkaline solution.

Separation techniques as filtration and sedimentation of the products will be used to investigate the differences when parameters as mixing/mixing temperatures/additives are changed. In addition analyzing techniques as Coulter Counter, XRD and SEM will be important methods for determination of crystal size distributions, phase distributions and morphology.

Most interesting is the precipitation of $FeCO_3$, FeS, $Mg(OH)_2$ (and $CaCO_3$).

***Co-supervisor: Ralf Beck***

**J-PA-2: Scaling and bulk precipitation of calcium carbonate at constant supersaturation**.

***Co-supervisor: Ralf Beck***

***Reserved for Margrethe Nergaard***

# Bioraffinering og fiberteknologi/Biorefining and Fibre Technology

## SM Førsteamanuensis Størker Moe

### SM-1: Kinetic study of the decrystallization of cellulose by concentrated mineral acid

One of the main obstacles for a wood-based biorefinery based on fermentation technology is the pretreatment and subsequent hydrolysis of wood polysaccharides into fermentable sugars. The strong acid process is an interesting process for pretreatment/hydrolysis, since it can be regarded as robust with regard to raw material choice and produces low amounts of sugar degradation products which can inhibit fermentation. Little has been published on the characteristics of strong acid decrystallization of lignocellulosic material, data which are necessary for industrial implementation of the process

The purpose of the work will be to investigate the hydrolysis and degradation of carbohydrates during decrystallization and hydrolysis of lignocellulosic material by strong acids, and fit these data to a simple model of the reaction behavior.

***Co-supervisor: PhD student Kando Janga***

### SM-2: Pretreatment of Norwegian Spruce using ethanol organosolv process to increase the efficiency of enzymatic hydrolysis of wood

To examine the effect of the ethanol organosolv process as a pretreatment method to produce ethanol from softwood lignocellulosic material. Ethanol delignification may be carried out alone or combined with previous steam explosion or hot water pretreatment which causes hemicellulose degradation/extraction and lignin transformation due to high temperature, thus increasing the potential of enzymatic hydrolysis. Different process parameters during ethanol pretreatment may be optimized like ethanol charge, temperature, reaction time and use of acid catalyst (acetic acid in place of sulphuric acid to avoid corrosion) to enhance the effect of organosolv pretreatment.

***Co-supervisor: Post. doc. Swarnima Agnihotri***

### SM-3: Torrefied pellets from Scandinavian forest residues for coal co-firing

In Europe a new pellet market for large-scale co-firing in coal-fired power plants has been created by governmental support measures (e.g. feed-in tariffs). For such purpose, Canada has become a major wood pellet exporter to the European market and more than 80% of wood pellets produced in Canada are shipped to Europe. From a logistics point of view, Norway is a good location from production biomass pellets from the European market.

Torrefaction is a promising pre-treatment option, improving the properties of biomass feedstocks in favor of combustion and gasification. Depending on applied operation conditions torrefaction will increase of the heating value per weight unit, improved the hydrophobic nature, improve grinding properties and increase uniformity and durability of the biomass. These changes may help to mitigate certain constraints related to co-firing of biomass with coal, such as size reduction of biomass (problematic due to its fibrous structure), storage (dry matter losses, fungi growth) and feeding.

The purpose of the project is to compare essential product properties of torrefied pellets made from Scandinavian forest residues with similar properties of typical wood pellets qualities used for the coal co-firing market today. Here essential product characteristics are moisture content, bulk density, ash content, grindability and biomass particle size distribution. The results will be used to evaluate the potential for Norwegian pellets production from forest residues for the European co-firing market.

The project will be a part of the research project PROFIT - Profitable bioenergy and paper production through innovative raw material handling and process integration. The practical work will be carried out in cooperation with PFI personnel.

***Co-supervisor: Research Scientist Kai Toven, PFI***

***Reserved for Børge Heggvoll.***

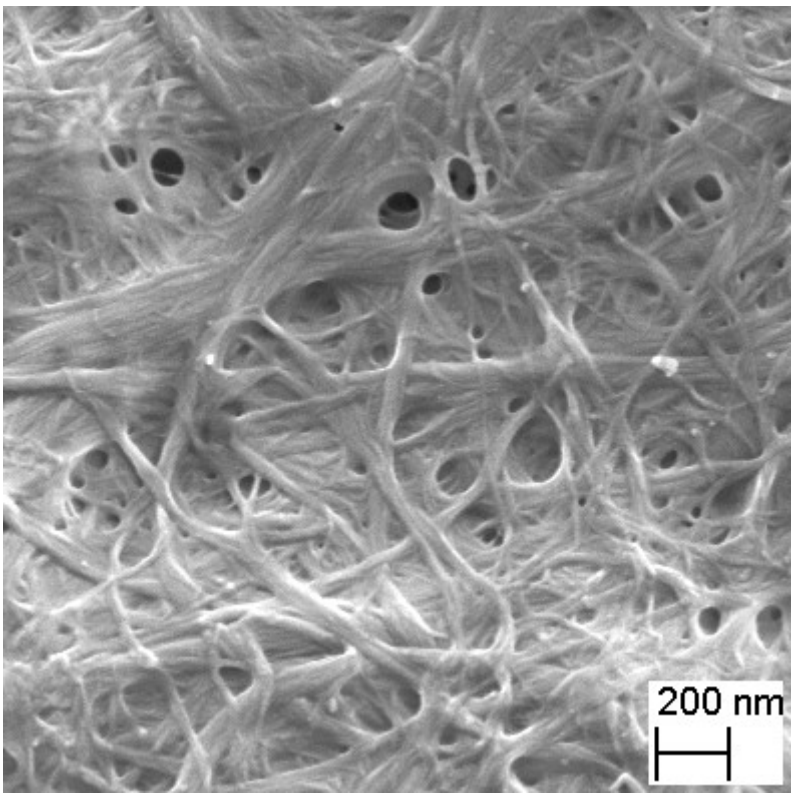
## ØWG Professor Øyvind Weiby Gregersen

### ØWG-1: Porous membranes / filters made of nanofibrillated cellulose

Nanofibrillated cellulose is a novel nano-material produced from cellulose fibres. The fibrils are composed of bundles of cellulose molecules giving a tread-like material with fibril diameters of typically 20 nm and with high aspect ratio and high specific surface area. The material retains many of the advantageous properties of cellulose fibres, such as the high strength and the ability to adhere to each other and make strong inter-fibril bonds. The small dimensions and the large specific surface area open up for applications that may not yet be foreseen. Central applications may be within membranes used in e.g. osmotic power production, for purification of water or in filters for air pollution. For all these applications, thin and strong membranes / filters with defined pore size in the material are crucial properties.

TEMPO mediated oxidation and homogenization will be applied for preparation of nanofibrillated cellulose. Films and filters will be prepared from the various fractions of fibrils. The samples will be characterized with respect to strength and morphology.

***Supervisors at PFI: Senior research scientists Kristin Syverud and Gary Chinga-Carrasco.***




**Field-emission SEM of the surface of model films made of nanofibrillated cellulose.**