NTNU
Norges teknisk-naturvitenskapelige universitet

Fakultet for naturvitenskap og teknologi
Institutt for kjemisk prosessteknologi

Suggestions for masther thesis 2012

at

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Department of Chemical Engineering

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**

I:/ikp/3 UNDERV /Masteroppgaver2012/Samleliste Masteroppgaveforslag 2012

Katalyse/Catalysis Group

EAB: Professor Edd A. Blekkan

EAB-1: Chemical quenching.

The project idea is to utilize useful endothermic reactions to cool very hot reaction mixtures. Examples of processes where this can be of interest are pyrolysis (e.g. thermal conversion of methane to higher hydrocarbons) or entrained flow gasification of biomass or coal to syngas. In the latter case the principle is used by CHOREN in the second stage of their 2-stage biomass gasifier. The quenching agent used there is char that is recycled and gasified by the steam and CO2 in the syngas. The reactions consume energy and the gas is cooled. This saves oxygen and ensures good utilization of the heat. Similar methods are used in coal gasification, e.g in the ConocoPhilips's (E-gas) gasifier. We aim to investigate if light hydrocarbons (C2-C4) can be used for the same purpose. The work will involve experimental tasks, utilizing and modifying a high-temperature tubular reactor unit, as well as literature studies. Theoretical studies (modelling and simulation of the processes) are also of interest.

Cosupervisor: Torbjørn Gjervan

Reserved for Alexei Pylilo

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, investigating in detail a catalyst system for this demanding process. Key elements of the work are catalyst preparation and characterization, and activity and selectivity measurements in a dedicated experimental set-up.

Cosupervisors: Andrey S. Volynkin, Ilya. Gorelkin

Reserved for Virginie Herauville

EAB-3: Hydrotreating of bio-oils over metal-phosphide catalysts

The production of liquid fuels from biomass is a key feature of a future renewable energy system. Bio-oils can be produced by biomass pyrolysis, and would in principle not contribute to anthropogenic CO2 when combusted since they are part of a natural biological cycle.

A main issue is the high content of oxygen in bio-oils (up to 50%) This is undesirable due to a low energy content (low heating value), thermal and chemical instability, poor miscibility with other fuels and a tendency to polymerize and form "gums" or particles. Therefore, the removal of the oxygen is necessary to allow the practical use of these oils. The hydrodeoxygenation (HDO) of oils is a hydrotreating process using hydrogen gas at high pressure. We want to study a new class of catalysts, metal phosphides for this process. The work is mainly experimental (catalyst synthesis and characterization, and catalytic experiments), supported by literature studies and theoretical considerations.

Cosupervisor: Sara Boullosa Eiras

***Reserved for* Christina Carlsen**

AH: Professor Anders Holmen

AH-1: Fischer-Tropsch synthesis on silisium carbide supported cobalt catalysts

Reserved for Sindre Håvik

AH-2:

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 synthesis of 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.

Supervisor: Prof. De Chen, Co-supervisor: Dr. Jun Zhu

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 by cracking process. 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 combined UV-Vis spectroscopy-MS and transient kinetic study on catalyst with different site density.

Supervisor: Prof. De Chen, Co-supervisor: Miroslave Surma

DC-3: Hydrogen production from biomass derived compounds by sorption enhanced reforming

Sorption enhanced reforming (SER) is a promising process to overcome the thermodynamic constrains and to reach one-step hydrogen production with high purity and yield from biomass derived compounds. The CO_2 high temperature acceptors and catalysts are installed together in the reactor. We have long worked on nearly pure hydrogen production by SER from biomass derived ethanol, glycerol, crude glycerol, sorbitol, glucose, synthesis gas from biomass gasification and crude biomass. There has been an excellent record of project and master projects on this topic, where four students worked on the topic, and each has at least one publication on high ranked journals based on their work. The present work will focus on the hydrogen production from bio-oils, which can be produced by fast pyrolysis of biomass. The project involves catalysts and sorbents synthesis and test in as fixed bed reactor using probe molecules such as acetic acid, acetone and aromatics.

Supervisor: Prof. De Chen, Co-supervisor: Dr. Javi Fermoso Dominguez

DC-4: Simulation of sorption enhanced steam methane reforming for use in technology assessment of pre-combustion CO_2 capture

There is a cooperative project with Det Norske Veritas (DNV). DNV has recently released a recommended practice for the qualification of CO_2 capture technologies. Currently DNV is expanding upon this by developing simulation platforms and guidelines for the verification and validation of process simulations. The specific scope of this work is within simulation of new developments in Pre-combustion CO_2 capture processes, and more specifically Sorption Enhanced Steam Methane Reforming (SESMR).

In order to precisely predict the performance of the whole process for the new concepts such as SESMR, it is necessary to have a well established base-case model representing the new reactor concept. As for the main focus of the project and master student project, a specific task on the mathematical reactor modelling for SESMR process is suggested. The proposed individual mathematical reactor model will be linked to the process model developed in Aspen Hysys.

The task will mainly include the following activities:

1. Literature survey on the topic
2. Selection of proper modelling tool (Matlab/Aspen Adsorption/Aspen Plus/Aspen Hysys) based on experience gained in the development of similar in-house models and final purpose of this work

3. Gathering necessary input data for (and / or developing sub models for the estimation of) the model e.g. equilibrium and kinetic constants for a selected sorbent and based on successful experimental data as well as heat and mass transfer properties of the system
4. Development of the base-case model using the selected tool
5. Verification and validation of the simulation results and integration of the model in the whole process model developed in Hysys (impact study)

Tasks 1 and 2 may be performed within the framework of the autumn project and in order to gain insight into SESMR in general and further develops knowledge on the development of reliable and meaningful inputs for the model. The project is thought to continue with a master thesis, where the scope will be to extend the work done in the autumn project, by development of the reactor model and the impact study through integration with the whole process model.
This project is proposed for a candidate who are interesting to take a summer job in DNV and continue both project and diploma work afterwards.
Supervisor(s): Prof. De Chen, NTNU, Hamidreza Bakhtiary, DNV

DC-5: Kinetic study of chain growth in F-T synthesis

Fischer-Tropsch synthesis is the key process in the production of liquid fuels from natural gas, coal and biomass. The reaction mechanism has long been the central research topic. However, the mechanism for the chain growth in the F-T synthesis is still in debate. The present work will deal with a steady-state isotopic transient kinetic analysis combining a detailed kinetic study at mediate CO pressures to elucidate the chain growth monomers. The project includes also the synthesis of Co nanoparticles with controlled size and shapes. The kinetic study will be performed on the resulting materials to gain a relationship between the properties and catalytic performance.
Supervisor: Prof. De Chen, Prof. Anders Holmen, Co-supervisors: Dr. Jia Yang, Dr. Jun Zhu and Prof. Erling Rytter

DC-6: Synthesis of graphene-carbon nanotube composite and applications in CO_2 capture at relatively low temperatures

Recently we have developed a new graphene-CNT composite where CNTs separate the single graphene sheet. The composite has a high surface area (400-500 m2/g) and macroporous structure, and high mechanic strength. The proposed project will deal with a modification of the carbon surface on a purpose of selective CO_2 adsorption at a wide range of temperatures. The kinetic study of CO_2 capture and regeneration will be performed in a TGA.
Supervisor: Prof. De Chen, Co-supervisors: Fengliu Lou, Prof. Erling Rytter

DC-7. 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. The electrode will be tested in electrochemical station as supercapacitors on a purpose of energy storage in chemical bonds with conductive polymer.
Supervisor: Prof. De Chen, Co-supervisor: Fengliu Lou

MR: Professor Magnus Rønning

MR-1: 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.

Supervisor/ co-advisors: Magnus Rønning/ Asmira Delic

MR-2: 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. The project deals with characterisation 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 close collaboration with Statoil and SINTEF.

Supervisor/ co-advisor: Magnus Rønning/ Georg Voss

MR-3: Hydrothermal synthesis and characerisation of Cobalt Fischer-Tropsch catalysts

Supported cobalt catalysts are widely studied and applied for conversion of synthesis gas in low temperature Fischer-Tropsch synthesis. The master work will include synthesis, characterisation and testing of FT catalysts. Particular focus will be given to catalysts prepared by hydrothermal synthesis. The master will be carried out at Statoil Research Centre and NTNU.

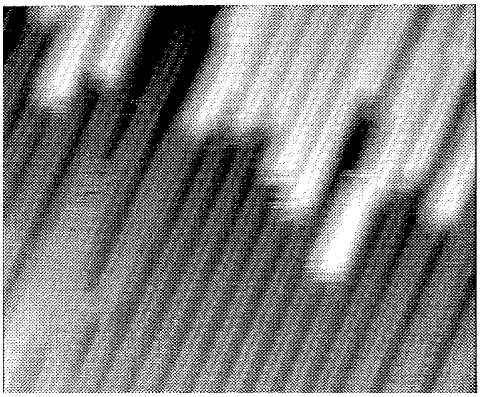
Supervisor/ co-advisors: Magnus Rønning/ Statoil: Erling Rytter/Sigrid Eri

The project is reserved for Nina T Gynnild

HJV: Førsteamanuensis Hilde J. Venvik

HJV-1: Adsorption of alkaline metals on cobalt single crystal surfaces

Cobalt based catalysts are important in converting synthesis gas (CO + H2) derived from natural gas, coal or biomass into liquid fuels through the Fischer-Tropsch-synthesis. Small amounts of alkali metals present in the reactant mixture have, however, been found to affect the activity and selectivity of the catalyst. katalysatorens aktivitet og selektivitet. This is typically the case if the feedstock is biomass, since these elements may exist in biomolecules. In the commercial application, the cobalt dispersed on a porous support, but investigations of well ordered single crystal surfaces under controlled atmosphere may provide insight to the adsorption and reaction phenomena on a molecular scale that may explain the observations made under realistic conditions.



The project concerns atomic scale experimental investigations of ordered cobalt surfaces through application of scanning tunnelling microscopy (STM) as well as other relevant techniques (XPS - x-ray photoelectron spectroscopy and , LEED – low energy electron diffraction, etc.). Small amounts of alkalis (Na, K) will be deposited on the cobalt surface in order to determine typical adsorption sites and structures. Thereafter, the effect of alkali deposits on other, Fischer-Tropsch relevant, phenomena may be studied, for example CO adsorption and Co-restructuring. The figure shows a

20 nm x 15 nm STM image published by the supervisors on how a Co(11-20) surface was restructured into a new, ordered arrangement upon CO adsorption.

The MSc thesis is offered in a collaboration between Dept. of Chemical Engineering (IKP), and Dept. of physics (IFY), and is well suited for students specializing in *Nanotechnology for materials, energy and environment* as well as *Catalysis/Chemical Engineering*, with and interest in experimental investigations.

Supervisor: Professor Hilde J. Venvik, Dept. of Chemical Engineering (IKP), (Hilde.Venvik@chemeng.ntnu.no)
Co-advisors: Prof. Anne Borg, Dept. of Physics (IFY), Dr. Lars Erik Walle, IFY, Dr. Bjørn Chr. Enger, IKP.

Kolloid- og polymerkjemi/Colloid- and Polymer Chemistry

JOHS: Professor Johan Sjöblom

JOHS-1: Thermal Memory Effects

A fundamental investigation will be performed to assess thermal memory effects in complex petroleum fluids. An ethyl acetate extraction process will be performed to isolate the colloidal fraction from a complex petroleum fluid, and the various polarity fractions of the colloids will be determined. Separate model fluids will then be formulated containing one or more polar fractions as well as the paraffinic content of the initial complex fluid. Thermal memory effects will be determined using pour point determination tests as well as by rheological investigations. The role and function of the various polar colloidal fractions in the thermal memory mechanism will thereby be elucidated.

Cosupervisor: Dr. Kristofer Paso

JOHS-2: Paraffin Inhibition Mechanisms

A fundamental investigation will be performed to identify the mechanisms of polymeric inhibitors for waxy crude oil systems. A double wall glass vessel will be constructed with excellent thermal control. Waxy oils will be formulated with common paraffin inhibitor polymers. After crystallization, samples will be taken from the vessel and analyzed by FTIR analysis. Peak changes associate with the carbonyl bond will be followed to allow accurate determination of liquid phase polymer concentrations. In addition, FTIR analysis will allow determination of the final environment of the polymer chains, allowing determination of the mechanisms of paraffin inhibitor polymers.

Cosupervisor: Dr. Kristofer Paso

JOHS-3: Cloud Point Depressants/Rheological WAT determation

A fundamental investigation will be performed to identify the mechanism of cloud point depressants in model oil systems. A double walled glass vessel will be constructed with control of thermal and mixing conditions. Waxy oil systems will be formulated with and without polymer additives. The model oils will be loaded, dissolved, cooled, and sampled for GC analysis with linear and step-wise cooling profiles. Manipulating the thermal profile will allow elucidation of whether cloud point depressant mechanisms are thermodynamic or kinetic in nature. The results will be corroborated by WAT measurements using rheology, which will also serve to elucidate the utility and best practices associated with rheological WAT determination.

Cosupervisor: Dr. Kristofer Paso

JOHS-4: Development of E-NMR

The project will sort under liquid-liquid separation at Ugelstad Laboratory and marks a pioneer impact in the field of NMR applications.

We have previously developed low-frequency NMR for determination of droplet sizes and level measurements for offshore separation

application. We have established for this purpose a program followed by 12 leading oil companies in the world. The level of the technology is documented

in a recent PhD (Nils Opedal) thesis. In order to further develop the competitive edge at UL and Antek A/S we have decided to develop E-NMR to monitor the

influence of an electrical field on droplet under simultaneaous monitoring by NMR. The MSc work will be to design a cell and do first pioneering measurements.

Good possibilities to patent the solution.

Supervisors: Sebastien Simone, Geir Sørland and Johan Sjöblom

JOHS-4: Purification of tetra-acid and characterization of its properties at the liquid-liquid Interface

Tetra-acid (also known as Arn) is a molecule present in petroleum crude oil at low concentration, typically the ppm level, which can precipitate in presence of calcium to form deposits. These deposits have an impact on oil production and can even lead to costly shut-down.

In order to understand the formation mechanism of these deposits, obtaining pure tetra-acid samples are required. The goal of this work is to improve the current process of preparation and purification of tetra-acid by preparative HPLC. Enough pure tetra-acid will then be prepared to study their interfacial properties by interfacial tension and interfacial rheology measurements.

This diploma project will be a part of the *Joint Industrial Program 2* project, with several central oil companies and chemical vendors as participants.

Supervisors will be Dr. Sébastien Simon and Professor Johan Sjöblom

GØ: Professor Gisle Øye

GØ-1: Interfacial characterisation of dispersed components in produced water

Produced water is water co-produced with oil and gas during petroleum production. Worldwide the average production of water is 3 times higher than the petroleum production, and the water content continues to increase as the oil fields become more mature. Pollutants like dispersed oil and solids must be separated from the produced water streams prior to discharge or reinjection, and efficient and reliable treatment processes are required. This means that it is necessary to understand the mechanisms that govern the separation efficiency at the molecular level, and the interfacial properties are crucial in this respect. The main objective in this project is to measure interfacial tensions and interfacial rheology between crude oil fractions and aqueous solutions. The interfacial properties will be related to the formation and separation efficiency of corresponding oil-in-water emulsions.

The project will be carried out in collaboration with an industrial consortium.

Supervisors: Bartlomiej Gawel/Mona Eftekhardadkhah and Gisle Øye

Reserved for Cathy Lesaint

GØ-2: Characterisation of dispersed components in produced water

Produced water is water co-produced with oil and gas during petroleum production. Worldwide the average production of water is 3 times higher than the petroleum production, and the water content continues to increase as the oil fields become more mature. Pollutants like dispersed oil and solids must be separated from the produced water streams prior to discharge or reinjection, and efficient and reliable treatment processes are required. This means that it is necessary to understand the mechanisms that govern the separation efficiency at the molecular level, and the interfacial properties are crucial in this respect. The main objective in this project is to determine the separation efficiency and drop size distributions of crude oil fractions dispersed in aqueous solutions.

The project will be carried out in collaboration with an industrial consortium.

Supervisors: Bartlomiej Gawel and Gisle Øye

Reserved for Dmitrij Viatkin

WRG: Førsteamanuensis Wilhelm R. Glomm

WRG-1: Smart nanoparticles for targeted drug delivery

Combining nanoparticles with pharmaceutically active compunds such as small drug molecules, peptides, enzymes and antibodies holds great promise in developing “smart” drug delivery vectors with superior performance and selectivity. The successful design of these new materials depends on an understanding of how the pharmaceutically active compound interacts with the nanomaterial, and to which extent the components exhibit emergent properties, i.e.; whether or not the nanoparticle construct has (desirable) properties not found in either the nanoparticle or pharmaceutical compund alone. In addition to carrying a pharmaceutically active compund, the nanoparticle core can act as a diagnostic tool; either optically (by

using noble metal nanoparticles) or provide enhanced contrast in MRI measurements (by utilizing magnetic nanoparticles), or a combination thereof.

In this project, various nanoparticle vectors will be synthesized, and the properties will be screened based on stability in biological media, optical and/or magnetic properties, and, where applicable, functionality of the construct. The prospective nanoparticle constructs will primarily be investigated using experimental techniques available at the Ugelstad Laboratory.
Main subject teacher: Wilhelm Glomm, IKP, e-mail: glomm@nt.ntnu.no, Phone: 73 59 41 58
Co-supervisor: Sina Maria Lystvet (IKP)

WRG-2: Membrane interaction of protein-nanoparticle constructs

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. During the last decade, there has been an exponential increase in the research on and fabrication of protein-nanoparticle constructs. Recent studies have shown that the protein-nanoparticle constructs may possess emergent properties, i.e.; properties not found in either the nanoparticle or protein alone. An example of emergent properties is increased membrane interaction and destabilization of lipid films. While this is a highly desirable property for protein-nanoparticle constructs developed for targeted drug delivery, it is also a growing concern given the possible negative impact on health and environment. An understanding of the underlying mechanisms and interaction kinetics as well as how protein-nanoparticle constructs affect lipid membrane models is therefore crucial to the field of nanotoxicology. In this project, lipid interaction and interfacial activity of protein-modified nanoparticles will be investigated using experimental techniques available at the Ugelstad Laboratory (spectroscopic techniques and interfacial measurements). 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-supervisor: Sina Maria Lystvet (IKP)

Forslag sendt til NTNU fra Forsvarets forskningsinstitutt (FFI) v/Bernt B. Johnsen (telefon: 63807834, e-post: bernt.johnsen@ffi.no)

WRG-3: Nanocomposites – polymers with nanoparticles

Forslag sendt til NTNU fra Forsvarets forskningsinstitutt (FFI) v/Bernt B. Johnsen (telefon: 63807834, e-post: bernt.johnsen@ffi.no)

The properties of polymer materials can be altered or tuned by addition of different nanostructures, such as carbon nanotubes, nanofibers or other nanoparticles. Using nanotechnology, plastics, composites or adhesives with improved materials properties can be fabricated, which is of significant importance within aeronautics, missile- and space industry, where a lot of research is focused on lightweight materials with outstanding mechanical properties.
In order to optimize the properties of the nanocomposites, it is necessary to obtain a system with a high degree of dispersion of nanoparticles within the polymer matrix, as well as to ensure polymer-nanoparticle compatibility. Obtaining an understanding of how the nanoparticle surface chemistry affects the mechanical properties of the nanocomposites is of crucial importance. FFI (The Norwegian Defence Research Establishment/Forsvarets Forskningsinstitutt,) can offer two related but separate projects within this area:

1. The main focus of this project is on chemical surface modification of commercially available carbon nanotubes, and the effect of this surface modification as the nanotubes are used as reinforcements in a polymer.
2. In this project, the main focus will be on how the mechanical properties of a polymer are altered upon addition of carbon nanotubes or aluminum nanofibers. Particularly how maximum dispersion can be obtained, as well as the effect of various surface modfication of the nanotubes/fibers. Relevant characterization techniques include mechanical testing, chemical surface characterization and various microscopic techniques for microstructure assessment (ligh microscopy, TEM, SEM

and AFM). FFI has ongoing activity within this field, and will collaborate closely for the duration of the project.

Subject teacher: Wilhelm Glomm, Institutt for kjemisk prosessteknologi, NTNU, (wilhelm.glomm@chemeng.ntnu.no), Co-supervisor: Bernt B. Johnsen, FFI (bernt.johnsen@ffi.no)
Reservered for Signe Marie Nielsen Stavnes

WRG-4: 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: Catalytic combustion control

The overall aim is to find a better way of controlling a given combustion process.
The autumn project (2011) has focused on developing a simple Matlab models that shows the observed hotspot behavior. In the Mater project this model should be extended to include all the parts of the process and to study the control of the process.
The work is in cooperation with Perstorp (Krister Forsman).
Co-supervisor: Johannes Jäschke
Reserved for Carina Renee Nerland

SIS-2: Optimization of processes using "self-optimizing" variables

This project is motivated by our difficulties in optimizing LNG (liquefied natural gas) processes, but also other (simpler) processes may considered.

Steady-state simulation and optimization of LNG processes is difficult because of tight integration and small temperature differences between the streams. For example, the UniSim has large problems in converging when trying to optimize the operation of a given network. One possibility is to let Matlab do the optimization and UniSim the simulation. The focus in this project is on finding the best variables to specify in UniSim. Another approach is to use dynamic simulation for finding the steady-state solution. Also in this case the selection of good "self-optimizing" variables is critical.
Co-supervisors: Jophannes Jäschke (postdoc) and Vladimiros L. Minasidis (PhD student)
Reserved for Roald Bræck Leer

SIS-3: Optimal operation of networks using self-optimizing control

The idea of self-optimizing control is to achieve near-optimal control by keeping certain variables or variable combinations constant. For heat exchanger networks with parallel branches, we have developed a simple polynomial variable combination which we are considering to patent. The objective is to further study the method by considering specific applications, for example, to (a) crude oil preheating (Statoil Mongstad, Esso Slagentangen) (b) LNG processes (Statoil Hammerfest) , (c) chemical plant (Perstorp) or (d) district heating (Tiller). Matlab and Simulink will be used for simulations
Co-supervisor: Johannes Jäschke, postdoc
Reserved for Alexandre Leruth

SIS-4: Dynamic back-off for control of active constraints

To operate processes safely generally there are constraints which have to be observed. A typical examples for a safety constraint is the maximum allowable temperature in a reactor. Exceeding this constraint can lead to serious consequences, e.g. explosions.
At the same time, it often happens that the plant profit is maximised when a variable is at this constraint. Therefore it is desirable to operate the process as close to the constraint as possible. In practice, we will always have to back off a little bit from the constraint, because we want to make sure that we do not violate it, even if the the process conditions vary. At the same time, we want to minimize the back-off, because it causes economic loss.
The goal of this project is to study how the back-off can be adapted to dynamically changing operating conditions. The principal idea is to impose large back-off when the variable value changes fast, and little back-off when the variable changes slowly or not at all.

The student should like to work with matlab and have some knowledge about simulation of differential equations.
The tasks are

- Literature review
- Set up a small dynamic model

- Find a law which dynamically adapts the back-off to the rate of change in the variable
- Simulate a batch reaction process as a case study

Co-supervisor: Jophannes Jäschke, postdoc

SIS-5 Flexible/optimal steady-state backoff for unconstrained variables to avoid infeasibility

To operate processes safely generally there are constraints which have to be observed. A typical examples for a safety constraint is the maximum allowable temperature in a reactor. Exceeding this constraint can lead to serious consequences, e.g. explosions.
Variables which are unconstrained under a certain set of operating conditions may reach a constraint under other conditions. To remain truly optimal in both operating conditions, the control structure has to be changed.
In practice, however, one would like to keep the control structure simple and to use one control structure for all operating conditions.
This project involves investigating under what circumstances a control structure can be found, which may not be truly optimal, but which does not have to be adapted to changing constraints.
We will consider the case of a linear plant and a quadratic objective function.

The student should like to work with matlab or some other programming language and have some knowledge in linear algebra
Tasks:

- Literature review
- Set up small examples and find control policies, which give an acceptable loss
- Derive theoretic results about how much loss has to be accepted when using a single control structure for all operating conditions

Co-supervisor: Jophannes Jäschke, postdoc

SIS-6: 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 and the multiphase group at the Department of Energy and Process Engineering (Prof. Ole Jørgen Nydal).

6.1: 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 usability.
Co-supervisor: Esmaeil Jahanshahi (PhD student)

6.2: 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-7: Studies on control of distillation columns (in cooperation with Statoil/Gassco at Kårstø)

The project is motivated by operation of distillation column far from original design, and with significant variation in feed rates and feed composition at Kårstø gas prosessing plant. Significant variation in feed results in significant variation in the process dynamic and in challenges with oscillation in the regulatory control layer (PID) and in the supervisory control layer (here: Model Predictive Control, MPC).

The objective is to systematic study the process dynamic at different feed rates and feed composition to improve the understanding and, if possible, propose a way to use gain scheduling in PID-layer and/or MPC-layer. One approach would be use the SIMC PID tuning rules as a basis.

Matlab will be used in the initial phase to improve understanding, while Dspice dynamic simulator and MPC will primary be used in later phase for studying specific columns.
Reserved for Iakov Dolgov

SIS-8: Expected problems when pairing on negative RGA-elements
The basis for this project is that it is not clear what happens if one pairs on a negative RGA. This will be a mix between simuklation (in Simulink) and theory.

Background: Pairing on a negative steady-state RGA-element may give good decentralized control performance, but there are potential risks.
First, note that if one pairs on a negative RGA, then one cannot tune the controllers using independent designs (where each loop is tuned separately with the other loops in manual), because one would get instability when all loops are closed.
Second, consider sequential loop closing, which is probably more common practise. In this case, pairing on a negative RGA is claimed to result in instability, and the objective is to study this in more detail.

SIS-9: Optimality of PI and PID control
The objective is to study for which processes PI and PID control are best suited. It is well established that it works for first- or second-order processes with delay. To objective is to conform this rigorously and to consider also other processes. Subtasks

1. Define basis for comparison (combined performance and robustness measure)
2. Find optimal controller for a range of processes and compare with best PI/PID controller.

Cosupervisor: Chriss Grimholt

SIS-10: Simulation and control of pressure/flow networks using Matlab

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.
Reserved for Sebastian Roll

HP-2: Control lab rejuvenation : Distillation
Now some time ago, the department received 2.5 million NOK for the development of the felles lab and the control lab. Most of the units have been re-designed or updated and a couple of new ones have been

generated. We still need some more experiments and updating. Objective is to bring in novel and advanced instrumentation whilst at the same time widen the experiment domain.

Last year we have rebuilt the distillation columns and they are now department show cases having been upgraded from being just sheet-metal tube kind of look to shiny glass and aluminium constructs. The heat exchangers have been moved to the side making the overall construct to be close to industrial arrangements. Next we intend to make two columns to operate continuous, thus we need feed pumps and distillate and bottom product handling. Further we need to extend the control software to accommodate the new power control units and the units associated with the planned extension

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

HP-3: Control lab rejuvenation: Residence time distributions tubular reactor
Along the same lines as HP-2, we are in the process of building experiments around the theme of time-residence distributions. We are given a new cut-of-the-edge tubular milli-reactor of the type BASF is using for realising their new manufacturing concept. It will also involve a new optical distributed temperature measurement based on a fibre-bragg optical sensor sampled by a laser.

HP-4: Control lab rejuvenation: Residence time distributions toy box
Same as HP-3 but experiments are based on either salt-solution as tracer or ink-like substances. First being measured using conductivity measurements the second optical measurements.
This project is assigned.

HP-5: Control lab rejuvenation: A toy box
Motivation is the same as above, but aim 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-6: 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-7: 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.
A first master project was done last year in co-operation with Polimi (Milano), the leading chemical engineering department in Italy.

Global aim is to furnish a systematic way of exploring the possible faults in a system, a subject of great interest to industry.

HP-8: 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-9: 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-10: 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.

HP-11: Theoretical study of thermodynamics

Gibbs had the insight, Caratheodori did the first pass on the mathematics (1909) and it keeps on popping up here and there. Today it is known as contact geometry, a branch of analytical differential geometry that provides a complete framework for the representation of thermodynamics. There are a number of open questions one of which is, if this entry point is easier than the classical approach. The description is explored and applied on extreme scales such as quantum mechanical systems as well as on black holes. Thus it aught to describe also chem engineering systems very elegantly....

HP-12 Nano-macro: System representation suitable for multi-scale modelling

Background

Future modelling tools are to construct models based on built-in ontologies. These ontologies are a representation of the underlying physical and if appropriate chemical biological concepts. The technical representation of this knowledge in terms of software is of secondary importance. Primary stands the exploration of what level of the physical concept framework is being used and how it is formulated. Recent years have seen a renaissance of geometrical methods, in particular a twin to the Hamiltonian mechanics is evolving in contact geometry, which has its origin in Gibbs' and Carateodori's publications being further developed in theoretical and mathematical physics in the past one to two decades trying to digest the intermediate burst appearing in the 70ties.

The Project

The contents of the project is loosely defined on the application side. The research is to go into exploring the feasibility and use of these theories to construct a theoretical “jacket” that can be used as a template for the construction of multi-scale processes. The fundamental nature of the theory makes us hopeful that indeed this will be the case and publications in the theoretical physics area indeed seem to confirm the trend. Physical example systems can be drawn from the literature. The selection is part of the project and will be done with the candidate.

In a first stage one will explore the theory, get familiar with the technical details, apply it to generic systems probably mainly focusing on the material description – thermo part. In the mean time literature research for a physical test system can be done aiming finally at applying the theory to the multi-scale system yielding a consistent mathematical description that bridges the scales properly with regard to the conserved quantities and provides conform expressions for the intensities.

HP-13: Thinking future biorefineries

The light has dawned on at least part of humanity that fossil carbon sources are limited and that the mined carbon is largely dispatched into the atmosphere. The issues around the composition of the atmosphere being observed these days are in order of magnitude more severe than other problems earlier being detected and to some degree also being handled, namely NOx and FCl compounds. Simply the order of magnitude and the fact that mostly the energy resources are attached to the C-houshold make it much more sever and more difficult to handle.

Projecting that humanity indeed does switch away from mined carbon resources and increasingly relies on carbon being in the biotope cycle, we believe that the currently taken policy of replacing fuel and feed stock for the classical chemical production is not rich enough to address the problem appropriately. This approach may result in some improvement but it certainly is too small of a step to make the overall system, these days being the world as a whole, a sustainable system. We believe that any lasting development will have to implement a policy that follows the paradigm:

Sustainability can only be achieve if the human activity remains within the biotope we are part of and when the time scale of usage and regeneration match.

And that we adjust the goals for the operations to:

Complex molecules should be retained and built on in contrast to breaking things down to what we consider currently base stock.

Whilst we have the technology to synthesise from base stock and purification, the retaining operation requires only separation. This should be more energy efficient and have less side effects, whilst though requiring more sophisticated processes, but with energy requirements being likely significant lower and thus secondarily also contributing to improve sustainability.

Research will have to start on exploring the existing technologies as they were developed on the early 1900s and technologies that are evolving in the bio-technology departments and institutes. This project is about exploring and summarizing the current knowledge in bio-mass treatiment for the purpose of generating user-marked chemicals. It may involve SINTEF.

TH-W: FørsteamanuensisTore Haug-Warberg

TH-W-1: High-pressure thermodynamics using the Murnaghan Equation of State
Background: In high-pressure solid-gas, solid-liquid and solid-solid equilibria there is the need for accurate equations of state for very compressed materials. Such equilibria are important for the understanding of geochemical reactions and for phase transitions taking place under extreme conditions like in high-velocity shock fronts. There are several equations of state being developed with these problems in mind, one of them is the Murnaghan equation (actually a whole family of equations built on the same assumptions).

Goal: 1) Scrutinize the Murnaghan equation to fully understand its assymptotic behaviour. 2) Find experimental data for a number of simple inorganics like carbon, alumina, quartz, calcite, calcium oxide, magnesium oxide, dolomite, etc. 3) Do parameter fitting of the equation. 4) Compare with experiments. 5) Employ the equation in thermodynamic equilibrium calciulations encompassing solid-solid phase transformations.
Prior knowledge and experience: The student must show an interest in computer programming and numerical mathematics, and must have a good background in physical chemistry and thermodynamics.
upervisor (NTNU):
Co-supervisor (Yara):
Reserved for: Stig-Erik Nogva

TH-W-2: Further development and use of the Yara Process Simulator (YASIM)
Background: In big chemical industries like Yara (one lof the largest fertilizer producers in the world) there is a constant need for process simulations and process calculations, spanning in complexity from simple Excel sheets to rigorous flowsheet simulations with Aspen, Hysys, Prosim, etc. The current problem is that there are few tools available that actually makes life easier for the engineer. Excel sheets very soon become too complex to develop and maintain, while flowsheet simulators have a steep learning curve and requires day-to-day use in order to bring increased confidence into the work of the engineer. Yasim represents an effort to make rigorous thermodynamic calculations available at a pace hitherto unknown to the process industry. The concept is fairly straight forward: A small calculation server written in Ruby (and wrapped into Python) is used to administrate the requests from the Python client, and to call rigorous thermodynamic DLL's in the background. The server allows for creating material streams, building mass and energy balances, solve equilibrium equations using a unique combination of analytic formulations and numerical solver, etc. The server is currently running in a beta-version which has proved to be very stable.

Goal: 1) Implement, possibly in co-operation with Yara, an object-oriented flow sheet module in Python for building up flowsheets and administer simple unit operations like heat exchangers, small distillation columns, valves, etc. The work shall be conducted with focus on flexibility and extensibility of the code. Solving the problems numerically is not the central issue. More important is the possibility of running the simulator in text mode, i.e. generating readable output of what has been specified and what remains to be calculated at each stage in the simulation. 2) Suggest strategies for representing flowsheets with recycle streams. 3) Suggest possibilities for doing dynamic simulation.

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.

Co-supervisor (Yara): Dr.ing. Knut Wiig Mathisen, Dr.ing. Volker Siepmann
Reserved for: Ivar Nesje

NS-B: Førsteamanuensis Nadi Skjøndal-Bar

NS-B-1: 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 Nadav Bar, expert in modelling and analysis of biological systems, and is assisted by a Phd candidate which will co-supervise the student to provide the Master student full support.
Further information call 94124 or email nadi.bar@ntnu.no
Reserved for

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.
Co-supervisor: Rafael Sanchez

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.
Co-supervisor: Jannike Solsvik
Reserved for Stian Tangen

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.
Co-supervisor: Jannike Solsvik

HS: Professor Hallvard F. Svendsen

Relatet to CO_2-capture:

1 HS-1: Kinetics in CO_2-amine systems
Faglærer/Veiledere: Hallvard Svendsen/Ardi Hartono etc.
The project is reserved for Mohammad Usman

2 VLE for the CO_2-amine systems
Faglærer/Veiledere: Hallvard Svendsen/Ardi Hartono etc.
The project is reserved for Saddam Hussain

3 VLE for amine systems
Faglærer/Veiledere: Hallvard Svendsen/Ardi Hartono etc.
The project is reserved for Rafiq Ahmad

4: Exhaust gas quality for CO_2 absorption, Test Centre Mongstad.
Faglærer/Veiledere: Hallvard Svendsen,NTNU/Rehan Naqvi TCM
The project is reserved for Fridtjof Finsnes Henriksen

5: VLE and thermodynamics for acid gas treating
Supervisors: Hallvard Svendsen (NTNU)/NN Statoil Rotvoll
The project is reserved for Anita Bersås, anitb@stud.ntnu.no

6: Degradation inhibitors for amine system (CO_2 capture)
Supervisors: Solrunn Johanne Vevelstad, Bård Hoff and Hallvard Svendsen
The project is reserved for Jørund Elvran, Dept of Chemistry NTNU

MH: Professor Magne Hillestad

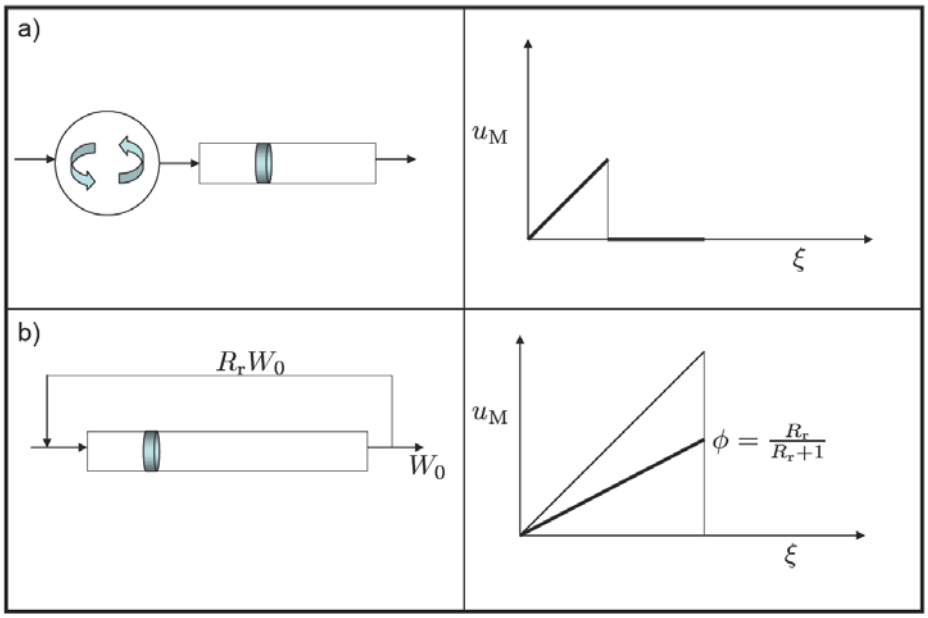
MH-1: The effect of operational parameters in a methanol plant
Statoil's methanol plant at Tjeldbergodden converts natural gas to methanol. The plant consists of an air-separation-unit (ASU), syngas production, methanol synthesis and raw methanol distillation. This project will focus on the methanol synthesis loop but also the syngas production is of interest.

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.

The continuation of this work for a master thesis will focus on new designs of the methanol synthesis.

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.
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. Application area can be on a free radical polymerization reaction where the objective is to design a reactor path that produces the desired molecular weight distribution (MWD). Review different ways of calculating the MWD, implement a method of calculating the MWD together with the entire kinetic model. Apply the model to find the optimal mixing configuration, initiator and monomer feed distrbution, heat transfer area and coolant temperature distribution in order to produce a desired MWD most cost effective way. Part of this will be suitable for a project work.
Co-adivor: PhD Student Paris Klimantos

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. Different technologies have been developed for syngas production unit such as steam methane reforming (SMR), autothermal reforming (ATR), gas-heated reforming and 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, such as slurry bubble column and fixed bed reactor.

Modelling of the GTL plant can be made in Hysys, Unisim or other systems. Model the FT unit will be by introducing a known kinetic model such as one given by Iglesia et al[1]. Compare different process configurations of syngas production in a GTL plant; perform a pinch analysis for optimal heat integration of the plant and make simple cost estimations for process evaluation.
Co-advisor: PhD student Ahmad Rafiee

MH-5: Energy considerations around an amine CO2 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-advisor: Karl Anders Hoff , SINTEF

MH-6: Evaluation of a North Sea oil platform using exergy analysis

The typical power consumption at a Norwegian continental shelf platform is around 10 MW to several hundred MW. Most platforms generate their own power with gas turbines and diesel engines. In 2008, gas turbines and diesel engines on oil platforms were responsible for 21 % of Norway's total CO_2 emissions [1]. Reduction in power consumption at the continental shelf is therefore an important challenge.

There is a need for a tool to evaluate the performance of such offshore platforms. CO_2 per produced oil is often used. However, different platforms have different operating conditions. Exergy efficiency is an alternative performance parameter where operating conditions are taken into account. Also, by doing an exergy analysis, one can indicate the potential for reduction in power consumption in the process.

Based on data provided by Statoil, a HYSYS model of the oil and gas processes of an offshore oil platform will be established. An exergy analysis will be performed, giving the exergy efficiency and indicating irreversibilities in the process.
[1] Statistics Norway, Statistisk Sentralbyrå. Emissions of greenhouse gases. 1990-2008*.
http://www.ssb.no/emner/01/04/10/klimagassn/ [29.04.10].
Coadvisor: PhD student Mari Voldsund, Department of Chemistry

MH-7: Sensitivity analysis of process simulations for CO_2 absorption.

To cater a growing energy demand and address the challenges posed by climate, new energy processes are being explored and developed. A critical aspect in this development is to demonstrate technological feasibility of the proposed concept. To predict and demonstrate technological feasibility, process modelling and simulation often is performed. Simulating these new processes requires sound knowledge on the fundamentals of the proposed technology as it often involves developing new models and tools.
Det Norske Veritas (DNV) has recently released a recommended practice for the qualification of CO_2 capture technologies. Currently DNV is expanding upon this by developing simulation platforms and

[1] E. Iglesia, S.C. Reyes, S.L. Soled, Reaction-Transport Models and the Design of Fischer-Tropsch Catalysts, Exxon Research and Engineering Company, Annandale, New Jersy, in: E.R. Becker, C.J. Pereira (Eds.), Computer-aided design of catalysts, New York 1993, pp. 199-257

guidelines for the verification and validation of process simulations. The specific scope of this work is within simulation of CO_2 absorption processes. For the modelling and simulation of CO_2 absorption processes there are two general pathways, namely the equilibrium based approach and the rate-based approach. The former approach is perhaps the most common, but it is also the one that is the least rigorous since it does not explicitly account for mass/heat transfer and chemical reactions at the gas/liquid interface. Instead these models relate the liquid and vapour phase states by assuming physical, chemical and thermal equilibrium between the bulk liquid and vapour phases. The predictability of equilibrium based models can be improved by incorporating tray efficiencies, but when it comes to scale-up the usage of tray efficiencies may be error-prone, since these are based on historical plant data which may not be valid for the new design. For the rate-based approach, the reactions and transport phenomena are accounted for in the contactor model framework. The model equations will thus be more challenging to treat numerically. But since the models in a more direct way accounts for the phenomena occurring in the system, they may be applied to any contactor without relying on plant data such as tray efficiencies.

Due to the increased level of rigour and detail in the sub-models, it is recommended that a rate-based modelling approach is used as basis for the project work. A possible platform for the project could thus be the Aspen Plus (Ratesep) simulation package. Any mathematical model of the real world – in this case a gas/liquid contactor will never be better than the data provided to the model framework. Rate-based contactor models require sound sub-models for e.g. thermodynamics, mass/heat transfer, kinetics and hydraulics. On the next level the models rely on proper correlations for physical properties such as densities, heat capacities, viscosities etc. The primary target of this work will be to establish a base-case simulation platform in e.g. Aspen Plus and further utilize this in order to quantify the impact of different sub-models on the overall simulation results. The proposed tasks are summarized in detail in the bullet points below.

- Develop a rate-based simulation platform for a base-case CO_2 absorption process in e.g. Aspen Plus
- Develop understanding of and document main sub-models in the model framework (i.e. flow model, mass transfer, kinetics, thermodynamics etc.)
- Compare sub-models and physical data with available experimental data
- *Investigate impact of different sub-models, and physical data on simulation results.*

It seems natural that the autumn project is used to gain insight into CO_2 absorption in general and further develop knowledge on the different sub-models, and how they are linked together. The project is thought to continue with a master thesis, where the scope will be to extend the work done in the autumn project, by performing a higher level sensitivity analysis.

Co-supervisors: Prof. Hallvard Svendsen, NTNU and Erik T. Hessen, DNV

MH-8: Modeling and model fitting of CO2 adsorption/desorption on a solid acceptor.

The project will involve modeling (dynamic) of mass and energy transfer in a solid particle and using laboratory data to identify adsorption and desorption kinetics.

The project is in cooperation with Professor De Chen.

M-BH Professor May-Britt Hägg

M-BH-1: Investigation of new polymeric membranes with controlled architecture for CO_2 capture

The focus of the project consists on screening of new materials as new polymeric 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 for gas separation with focus on CO_2 capture from flue gas and natural gas sweetening.

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. AFM investigations will be used in cooperation with Nanolab.

The membranes will be investigated by single gas permeation, CO_2, CH_4 and N_2. The gas permeation experiments will be performed under different controlled parameters: such as pressure and temperature. Gas sorption will be performed using CO_2 and N_2 and the results will be correlated with gas permeation experiments.
Membranes presenting the best separation properties will be further investigated by mixed gas permeation, synthetic mixture simulating flue gas composition. The influence of gas composition and humidity of the gas will be investigated for selected membranes.
Co-supervisor: Dr. Marius Sandru
Reserved for Marie Prache

M-BH-2: Preparation of PVAm/PSf composite hollow fibers for flue gas applications

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.
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 spinning and coating with a selective layer of PVAm followed by a protective coating. A focus of the project will be to investigate the possibility of spinning hollow fibers by using different polymer blends. The membranes will be investigated by scanning electron microscopy (SEM), gas permeation (before and after coating), IR spectroscopy and DSC.
Different parameters will be optimised to obtain by spinning highly permeable and defect free hollow fibers. One main focus of the project will be the study and optimization of 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.
Co-supervisor: Dr. Marius Sandru
Reserved for Petra-Kristine Johannessen

M-BH-3: Testing and optimization of PVAm/PVA blend membranes for biogas upgrading

This project will focus on the testing and optimizing of polyvinylamine/polyvinylalcohol (PVAm/PVA) blend membrane for biogas upgrading. The objective of this project is to develop a high performance membrane biogas upgrading. Based on the prepared PVAm/PVA fixed-sit-carrier (FSC) membranes, process simulation will also be conducted to evaluate membrane separation performance and process feasibility using HYSYS and economic cost estimation

The scope of this work can be specified as follows:

1. Permeation tests of the blend FSC membranes at different pressures (2bar, 5bar and 10bar). The membranes will be prepared in various conditions with various thicknesses. The tests will be performed in an advanced mixed gas permeation rig with a humidity regulator and an automatic operation monitoring and controlling system.
2. Optimization of the membrane preparation conditions based on the membrane separation performance at elevated pressures. The effects of cross-linking temperature and membrane thickness will be investigated and the optimized membrane preparation condition determined.
3. Characterizations of the blend membranes using SEM and XRD.
4. Spinning and coating hollow fiber FSC membranes
5. Hollow fiber FSC membrane test based on gas permeation measurement
6. Conceptual design and process simulation for biogas upgrading process.

Co-supervisor Dr. Xuezhong He
Reserved for Evind Berstad

M-BH-4: Testing and optimization of PVAm/PVA blend membranes at high pressure

This project will focus on the testing and optimizing of polyvinylamine/polyvinylalcohol (PVAm/PVA) blend membrane for natural gas sweetening at high pressures. The objective of this project is to improve the target membrane to be more resistant at high pressures (up to 80bar) without the loss of the CO_2 separation efficiency. Carbon nanotubes (CNTs) are considered as the nano-fillers in making the PVAm/PVA blend based nanocomposite membranes. In addition, the nanofiltration supported hollow fiber membrane will also be prepared and to be tested for high pressure natural gas sweetening.

The scope of this work can be specified as follows:

1. Permeation test of the CNT-blend membranes at high pressures (10bar, 20bar, 40bar, 60bar, 80bar). The membranes will be prepared in various conditions with various thicknesses. The tests will be performed in an advanced high pressure pilot scale rig with an automatic operation monitoring and controlling system.

2. Optimization of the membrane preparation conditions based on the membrane separation performance at high pressures. The effects of cross-linking procedure, support membrane, membrane thickness will be investigated and the optimized membrane preparation condition determined.

3. Spinning and coating hollow fiber membranes, and membrane test will also conducted at high pressure for natural gas sweetening

4. Characterizations of the blend membranes using SEM and other techniques.

Co-supervisor: Dr. Xuezhong He

Reserved for Anders Sørheim

M-BH-5: CO_2 separation from flue gas by FSC (fixed-site-carrier) membranes – Investigation on effect of polymer purity and process parameters on CO_2 separation in lab scale & pilot scale set-up

An excellent FSC (fixed-site-carrier) membrane for CO_2 capture has been under active development in MEMFO group (IKP, NTNU). The membrane is composed of CO_2 selective skin layer of PVAm (polyvinylamine) cast on a suitable support (for example, polysulfone, etc.).

The PVAm is prepared from commercial PVAm solution which contains about 10% impurity. The commercial PVAm has to be hydrolyzed and re-crystallization into pure solid polymer in order to be used for membrane material. It is expected that CO_2 separation performance can be further enhanced if the purity of the PVAm is enhanced. Meanwhile, it is also important to obtain PVAm of constant good quality through a standardized method which includes all related procedures such as hydrolysis, re-crystallization, casting solution on support, etc.

For further scale-up development of the FSC membrane process, a pilot scale membrane test set-up has been constructed and began to operate recently. The membrane performance from lab scale set-up needs to be confirmed at pilot scale set-up at first and then the performance dependency on various process parameters can be further studied at pilot scale set-up such as gas flow rate, pressure, temperature, etc.

In this project, the followings will be the major objects:

1) Investigation on optimized of PVAm preparation method for membrane use (hydrolysis, purification, casting, etc.) to be suggested as a standardized method
2) Investigation on effect of various process parameters on CO_2 separation performance at lab scale and pilot scale test set-up

Co-supervisor: Dr. Taek-Joong Kim

Reserved for Aristides Katto

M-BH-6: Forward osmosis membrane study on high temperature and crude oil systems Osmotic membrane pressure actuator (OMPA)

This project will be part of a collaboration with Statoil, and is a complete new way for looking at increased oil recovery from existing wells.

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. The FO membrane used at Telemark University College and Statoil were cellulose acetate and polyimide membranes. The property of the cellulose acetate membranes does not meet the requirements of high temperature conditions in the well and even though the polyimide material can withstand up to 300^{o}C initial testing revealed that the selective layer loosened from the support at higher temperatures. A screening of membranes to be used in OMPA was executed in 2010. It was found that a commercial available forward osmosis membrane with the properties to withstand high temperatures does not exist.

Scope of work (SOW)

The proposed project will be a follow up of a MSc-thesis performed spring 2011. The main part of Task 1 and 2 have therefore already been done, but some additional information for these two tasks will also be needed. The focus will therefor be on Tasks 3 and 4. The project will be performed in collaboration with Statoil.

The SOW is listed below in prioritized order. Task 4 may be considered as additional work.

1. ***A literature study*** on materials that can withstand temperatures up to 200^{o}C to be used for membrane development will be given together with a strategy on how to prepare the membrane. Other properties like potential durabilities and characteristics should be identified.
2. ***Membrane specifications*** for the group of selected materials will be identified using the well conditions from a specific field. An overview of potential 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. Other important characteristics that must be taken into account is the ability of a thinfilm selective layer to attach to the support at high temperature and the retention properties. The final membrane can potentially be a composite membrane consisting of an inorganic support coated with a thin film selective layer, a composite of two polymers, or an asymmetric membrane of one type of polymer. The various alternatives should be discussed.
3. ***Laboratory Testing of membranes*** to measure the properties of forward osmosis membranes will take place at the laboratory facilities at NTNU. The pore size, water flux, retention will be measured for commercial alternatives, likewise measurement of thermal stability (Tg) using DSC.
   The initial testing/characterizing of the membranes will be done in a RO cell – this is a usual way of doing the first scanning of materials.
4. ***Initial preparation/synthesis of new membranes*** that can withstand the conditions in a reservoir, i.e. temperatures up to 200 °C, pressure up to 200 bar and the chemical environment (condensate, saline reservoir water, H_2S, organic acids etc.) will be recommended. The membrane should be able to provide reversibility, acceptable resistance against fouling, have a long lifetime and high integrity.

Co-supervisor: PhD-student Inger Lise Alsvik

Not reserved

Crystallization

J-PA: Førsteamanuensis Jens-Petter Andreassen

J-PA-1: Nucleation kinetics of carbonate particles in natural gas production.
The off-shore production of natural gas in domestic fields like “Snøhvit” and “Ormen Lange” is performed by transport from the sub-sea production facilities in long low-quality steel pipe-lines. Large quantities of ethylene glycol are injected at the well-head in order to prevent the formation of gas hydrates during transport. The ethylene glycol is regenerated on-shore before being re-injected. The main problem in the regeneration process is the separation of small calcium (from reservoir) and iron (from pipe-line corrosion) carbonate particles from the MEG/water mixture. The size of the carbonate particles is a result of where and at which conditions of temperature and concentration the particles precipitate, as a result of the birth rate of the particles (the nucleation kinetics) and the crystal growth rate. The nucleation rate is calculated from determinations of the induction time and the crystal growth rate of carbonate crystals. The crystals will be analysed by SEM, powder-XRD and Coulter particle size measurements and proper training will be provided in these techniques. This assignment is part of a project sponsored by international gas producers and the results will be used in a simulator tool for MEG-loop installations.
Co-supervisor: Margrethe Nergaard
Reserved for Astrid Odland Barland

J-PA-1: Crystal growth kinetics of carbonate particles in natural gas production
The off-shore production of natural gas in domestic fields like “Snøhvit” and “Ormen Lange” is performed by transport from the sub-sea production facilities in long low-quality steel pipe-lines. Large quantities of ethylene glycol are injected at the well-head in order to prevent the formation of gas hydrates during transport. The ethylene glycol is regenerated on-shore before being re-injected. The main problem in the regeneration process is the separation of small calcium (from reservoir) and iron (from pipe-line corrosion) carbonate particles from the MEG/water mixture. The size of the carbonate particles is a result of where and at which conditions of temperature and concentration the particles precipitate, as a result of the birth rate of the particles (the nucleation kinetics) the crystal growth rate. The crystal growth rate is calculated from measurements of calcium (or iron) consumption in seeded growth experiments as determined by automated titration. The crystals will also be analysed by SEM, powder-XRD and Coulter particle size measurements. This assignment is a part of a project sponsored by international gas producers and the results will be used in a simulator tool for MEG-loop installations.
Co-supervisor: Ralf beck
Reserved for Charlotte Kleven Krossholm

J-PA-2: Precipitation during MEG-regeneration.
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 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.
Co-supervisor: Ralf Beck
Reserved for Torunn Kvam

J-PA-3: CO_2-capture in carbonate solutions with simultaneous precipitation

The project is to test different systems for CO_2 capture that results in precipitation and crystallization of solids to evaluate if this will improve the overall capacity and kinetics of absorption. During the later years it has been reported on CO_2-absorption in liquid systems where the reaction products crystallize during the capture process, like in the “Chilled Ammonia” process. The formation of solids is interesting if it can change the kinetics, improve the loading (how much carbon dioxide the solution can hold) or contribute to lower energy costs during regeneration of the absorbent. Like in any crystallization process the resulting particles (polymorphic composition, particle size and shape) will vary with temperature and the solubility/supersaturation of the compound that precipitates. The study will be performed in an automated lab-reactor system with probes that allow for the in situ observation particle size (FBRM) and shape (PVM, microscope). Typical absorption media will be carbonate salts of sodium and potassium, ammonia and amines. The solid products will be analysed by SEM and XRD.
Co-supervisor: Xiaoguang Ma

Bioraffinering og fiberteknologi/Biorefining and Fibre Technology

SM Førsteamanuensis Størker Moe

Production of biofuels and green chemicals from renewable resources is of increasing interest as an alternative to the current fossil based fuels and chemicals. Lignocellulosic biomass such as wood and agricultural crop residues (e.g. straw and bagasse) represents highly potential raw materials for producing e.g. fuel ethanol and green chemicals. These materials are of relatively low cost and plentiful supply and are considered very promising for replacing environmentally unfriendly fossil hydrocarbon raw materials.

The lignocellulosic biomass is chemically heterogeneous consisting mainly of the high molecular weight structural components cellulose, hemicelluloses, and lignin. Depending on the species, up to 80% of the lignocelluloses are polysaccharides which may theoretically be converted to e.g. fuel alcohols by fermentation. In contrast to traditional fuels, these biofuels do not contribute to the greenhouse effect, being a CO_2 neutral resource.

Pretreatment and enzymatic hydrolysis represents central process steps in the preparation of lignocellulosic biomass for further conversion. However these process steps currently form a significant part of production costs during conversion of lignocellulosics. Thus it is of significant economic interest to develop novel methods that will reduce pretreatment and hydrolysis costs.

A main challenge in the bioconversion of lignocellulosics is the recalcitrance of lignocellulosic biomass. Several pre-treatment processes have been developed aiming at deconstructing the lignocellulose by enlargement of the inner surface area, making the carbohydrates accessible to further hydrolytic treatment.

Hydrolysis of cellulose can be carried out by use of cellulolytic enzymes, chemicals or even steam. During enzymatic saccharification the accessibility of the substrate to the enzymes is of critical importance to obtain effective degradation of the cellulose.

SM-1: Decrystallization of lignocellulosic biomass using ionic liquids

Recently, treatment with ionic liquids has been presented as one possible way of processing lignocellulosic biomass. Selected ionic liquids have been shown to effectively de-crystallize the recalcitrant lignocellulosic biomass, giving effective solubilisation. Additionally, high lignin separation efficiency has also been documented. The drawback of ionic liquids is however their high cost, thus placing a high demand on their efficiency.

In this master project we aim to elucidate the solubilising effect of different ionic liquids on selected lignocellulosic raw materials, alone or in combination with other pretreatments. Focus of the work will be to:

i) optimise reaction conditions (temperature, time, wood:liquid ratio) for two selected lignocellulosic raw materials, using enzymatic hydrolysis yields as the main evaluation criterion
ii) elucidate the possibility to combine ionic liquids with other pretreatments (if time permits)

The work will be closely integrated with ongoing research project activities at PFI.
Co-supervisor: Karin Øyaas, PFI
Reserved for Jenny Kristin Håseth

SM-2: Organosolv pretreatment of biomass for biofuel and biorefinery applications

While organosolv cooking was originally developed as a pulping process for chemical paper fibers, it hasn't taken hold in industry for such applications. In more recent times, organosolv pretreatment is seen as a pretreatment option offering the possibility of enhancing the enzymatic digestibility of lignocellulosic

biomass while also producing a low-modified lignin byproduct with a potential for new lignin-based fine chemicals and materials.

The master project aims for the investigation of the organosolv process with regards to specific yields, cellulose digestibility by enzymes and the characterization of reaction products after the organosolv treatment.
The work will be closely integrated with ongoing research project activities at PFI.
Co-supervisor: Ingvild A. Johnsen, PFI
Reserved for Maren Seljenes Bøe

SM-3: Properties of torrefied pellets
Torrefaction is a promising pre-treatment option, improving the properties of biomass feedstocks in favor of combustion and gasification. At PFI, laboratory techniques have been established for biomass torrefaction, pellet production and pellets characterization in order to explore torrefied pellets as a new pellets quality.

The purpose of the diploma work is to produce torrefied wood pellets of four wood species and compare essential product properties with the same properties of traditional wood pellets.

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

The work will be closely integrated with ongoing research project activities at PFI.
Co-supervisor: Kai Toven, PFI

ØWG Professor Øyvind Weiby Gregersen

ØWG-1: Chip compressive cracking structure
Background
If wood chips are compressed axially during production, cracking and compressive plastic damage is done to the fibres. Results from refining trial indicate that such damaged chips may require 10% less energy corresponding to 200 kWh/ton less refining energy (1). For a paper mill like Norske Skog Skogn this corresponds to approx. 60 GWh/year or 12 mill NOK/year in savings. Further this type of chips absorb water and chemicals more easily, something which is a benefit in all bio-refinery operations for production of fuel or other products where wood is the raw material.
This new chipping technology is based on a patent (2).

The project
The change in the damage pattern of the chips depending on the chipping conditions is not yet much studied. The main task in the project is to use suitable electron microscopy techniques and light microscopy in combination with image analysis to characterize the micro and nano scale damage pattern through the length of chips (the damage is not uniform). The damage in the chips should be linked to the stress situation during chip cutting and the softening of the wood polymers due to temperature and moisture. If possible it is desirable to start developing a quick laboratory method for chip damage characterization. This may be based on absorption rate of liquids or on penetration of dyes in liquids. The project will be done in cooperation with the research group at Mid Sweden University who has patented the chipping technology together with Prof. Øyvind Gregersen.

References
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