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ved

Institutt for kjemisk prosessteknologi

Fagområder/-groups:

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

Katalyse/Catalysis Group

AH: *Professor Anders Holmen*

AH-1: **Effect of contaminants on the performance of alumina supported Co Catalysts**

Reserved for Andreas Helland Lillebø

AH-2: **Partial oxidation of methane by chemical looping**

Reserved for Cristina Azpeleta

EAB: *Professor Edd A. Blekkan*

EAB-1: **Model for prediction of mesophase based on LC-MS or NMR.**

The supply of light, sweet crude oil is diminishing, and in the future the industry will to an increasing extent be handling heavy crude oils. The production of nonconventional oil is growing (extra heavy oil, tar sand etc.), oils that are more difficult to produce, transport and process. To enable production, transport and marketing these oils need to be upgraded, involving reduced molecular size, reduced C/H ratio, reduced viscosity and removal of heteroatoms. Analysis and characterization of these oils are very challenging tasks due to the chemical and physical nature of the species involved. In collaboration with the Statoil Research center we work on characterization of heavy oils and products of heavy oil upgrading. A range of characteristics are important, in this project the formation of mesophase (anisotropic material) will be studied using LC-MS or NMR combined with statistical methods.

Supervisors: Edd A. Blekkan, Anne Hoff (Statoil).

Reserved Aderonke Badina

EAB-2: **Catalytic conversion of producer gas**

An attractive pathway to second generation biofuels is the thermochemical route, either via gasification or pyrolysis of biomass (e.g. wood). Gasification involves reacting the biomass with steam and/or oxygen at high temperature, resulting in a gas product (also called producer gas) that can be converted to fuels or chemicals in catalytic syngas-based processes. However, the producer gas needs cleaning, further reforming to convert hydrocarbons, and in some cases adjustment of the composition in order to fulfil the requirements of the downstream process. In this work we study catalytic reforming of hydrocarbons and tar and as well as water gas shift of realistic producer gas compositions. The goals include determining kinetic features, identifying the best catalysts and understand deactivation due to trace components in the producer gas.

Supervisors: Edd A. Blekkan, Espen Wangen

Reserved for Amin Osatiashtiani.

MR: *Professor Magnus Rønning*

MR-1: **Advanced characterisation of Fischer-Tropsch catalysts**

In situ characterisation methods are able to give information about catalysts and catalytic reactions at reaction conditions close to industrial processes. The Catalysis Group is using an increasing number of advanced *in situ* techniques for catalyst characterisation. Accessible techniques are spectroscopic techniques such as Raman, IR and UV-vis. In addition, the European Synchrotron Radiation Facility (ESRF) in Grenoble, France is frequently used for *in situ* X-ray spectroscopy (EXAFS) and X-ray diffraction (XRD). The project deals with *in situ* Raman, IR and X-ray spectroscopic studies of Fischer-Tropsch catalysts at industrially relevant conditions in terms of pressure, temperature and feed). Spending 1-2 weeks at the ESRF in France as a part of the project work is also an option. The work will include development of new experimental methods, optimisation and data analysis. The project will be carried out

in association with InGAP, a recently awarded centre for research based innovation, and in close collaboration with Statoil and SINTEF.

Supervisor/ co-supervisor: Magnus Rønning/Alexey Voronov

MR-2: New catalysts for preferential oxidation of CO in presence of hydrogen (PROX)

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

Supervisor co-advisor: Magnus Rønning/Tiejun Zhao

MR-3: Catalytic water purification

This project aims at the preparation and testing of catalyst supported on structured reactors coated with high surface area nanocarbon materials (NCM). The structured catalytic reactors will be used for catalytic water purification focusing on a different pollutant (nitrates, organics, etc). The purification will be performed by catalytic hydrogenation and oxidation processes. The properties of monolithic reactor coated with NCM, e.g. thin catalyst layer and mesoporosity, enable the control of the diffusion path and enhance the diffusion of reactant to catalytic sites. The objective is to achieve an intensification of the catalytic process in terms of improved selectivity, robustness, stability and performance while reducing energy requirements and by-product generation.

The project work will involve establishment of a continuous flow reaction set-up and the test various catalyst/structural reactor formulations in catalytic wastewater treatment. The project is part of a European programme (MONACAT, www.monacat.eu) involving European industry partners and universities.

Supervisor/ co-supervisor: Magnus Rønning/Estelle Vanhaecke

HJV: Førsteamanuensis Hilde J. Venvik

HJV-1: Catalyst for DME synthesis.

Dimethyl ether (DME) is the simplest ether, having the chemical formula of CH_3OCH_3 .

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

Supervisor, co-supervisors: Hilde Venvik, Anders Holmen, Fatemeh Hayer.

HJV-2: Microchannel membrane reactor for small scale hydrogen production

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

2 topics are envisaged:

A: We recently showed that the membrane's sensitivity to carbon monoxide (CO) could be changed (reduced) through a particular heat treatment, which has important implications for their applicability. The microchannel configuration is particularly suited for investigations of the phenomena that give this change. The topic involves studies of the effect of CO and CO₂ in the membrane microchannel configuration through experiments and modelling, as well as characterization of surface species present on the membrane during and after permeation experiments. The work will be carried out in collaboration with utføres i samarbeid med SINTEF Materials and Chemistry in Oslo.

Supervisor, co-supervisors: *Hilde Venvik, Thijs Peters (SINTEF), new PhD student*

B: The presence of the membrane and the microchannel configuration suggest optimum catalyst properties different than those of a "regular" MSR/WGS process, for which good kinetics at low temperature is often sought. Here, a regime of high membrane as well as reaction kinetics may be more suitable, where also the reaction equilibrium can possibly be shifted. The study involves synthesis, characterization and testing of new catalyst formulations with high MSR/WGS activity and good stability in the temperature range 300-400 °C, based on existing and new ideas.

Supervisor, co-supervisors: *Hilde Venvik, Edd Blekkan, new PhD student*

KM: Professor II Kjell Moljord

Two thesis proposal from Statoil R&D, Rotvoll

KM-1: Viscosity of heavy crudes due to asphaltenes

Description

The high viscosity of heavy oils is a challenge for the processing and handling of these crudes. To transport a viscous crude diluting with a naphtha or light crude or hot (>50-70°C) transport is required. Alternative means for reducing the viscosity represents a potential for a cheaper and easier processing of the crude.

The thesis will include investigate the role of asphaltenes on the viscosity of heavy crude oils by:

- 1) literature survey
- 2) experimental lab testing and analysis
- 3) process research for economical potential of using mild solvent deasphalting for viscosity reduction

The experimental testing involves solvent deasphalting of heavy crudes by a paraffinic solvent at different solvent-to-oil ratios and various operating conditions. The resulting deasphalted oil to be analysed for viscosity and other product properties. The thesis should conclude on the technical and economic potential of using a mild deasphalting process to improve the viscosity of a heavy crude oil.

Supervisor Statoil: *Jorunn Steinsland Rosvoll (jors@statoil.com)*

KM-2: Viscosity of diluted heavy crudes due to solvent properties

Description

The high viscosity of heavy oils is a challenge for the processing and handling of these crudes. To transport a viscous crude diluting with a naphtha or light crude or hot ($>50-70^{\circ}\text{C}$) transport is required.

The thesis will include investigate the role of different solvents on the viscosity and density of heavy crude oils by:

- 1) literature survey
- 2) experimental lab testing and analysis

The experimental testing involves blending of heavy crudes with different solvents (naphtha and condensate) to different concentrations. The viscosity and density of the blends shall be measured, and then a simple model shall be developed to predict the blending properties of the different solvents. There should also be looked into the correlations between viscosity and density for the blends.

Supervisor Statoil: *Marianne Haugan (mhaugan@statoil.com)*

Kolloid- og polymerkjemi/Colloid- and Polymer Chemistry

JOHS: *Professor Johan Sjöblom*

JOHS-1: Influence of paraffin waxes on emulsion stability

This work package will focus on the influence of paraffin wax on emulsion stability and separation. Paraffin waxes are non-polar molecules, and are not inherently interfacially active in the dissolved state. However, at temperature conditions below the Wax Appearance Temperature (WAT), paraffin waxes precipitate into micrometer-sized crystals or amorphous aggregates, providing solid particles onto which polar species such as resins and asphaltenes can adsorb. Hence, waxy crude oils effectively behave as Pickering emulsions at low temperatures when water is present. Interfacial electrostatic and van der Waals interactions between modified paraffin crystals can provide significant mechanical stability to an oil-water interfacial layer, and hinder emulsion separability. We plan on mechanistically investigating the interfacial activity of paraffin wax using techniques such as:

- Dynamic Interfacial Tension
- Critical Electric Field Emulsion Stability Cell
- Rheometry
- NMR (droplet size distribution)
- High precision densitometer (10^{-6} g/cm³)
- Langmuir-Blodgett Deposition & AFM (interfacial transfer and imaging)
- Oscillating Pendant Drop
- QCM (adsorption onto model surfaces)

The investigation will build up a fundamental understanding of the mechanistic behavior of paraffin wax crystals at the water-oil interface. Waxes containing linear, branched, and cyclic paraffin molecules will be utilized in the investigations. In addition, model fluids will be prepared containing various carbon number distributions, in order to gauge the effect of paraffin chain length. The wax activity will ultimately be mapped to the interfacial activity of the resin and asphaltene fractions. We aim to develop a complete aggregation model in which the synergistic effects of all SARA components are explicitly accounted for in terms of emulsion formation conditions, which will predict the emulsion stability and separability.

Co-supervisor: Kristofer Paso

JOHS-2: Microsimulation of the Hydrodynamics of Particle Suspensions: Sedimentation

The hydrodynamic and rheological properties of suspensions and emulsions are determined by the hydrodynamic forces exerted by the particles on the liquid and the electrostatic repulsion forces exerted between the particles themselves. The simulation method of Stokesian dynamics can be used to account for these forces and track the dynamic evolution of the microstructure of the particle suspension so that macroscopic physical properties of the dispersion can be calculated by ensemble averaging.

The scope of this work will be to introduce the student to the microsimulation technique of Stokesian dynamics and to learn the numerical methods employed to arrive at the solution. In particular, sedimentation of particle suspensions and emulsions will be studied. Furthermore, numerical methods for solving ordinary differential equations will be introduced to describe the electrostatic interactions between particles. The student will be expected to create and run original Matlab programs to obtain solutions to the given problem and to provide appropriate interpretation of the results. Consequently, a strong background in mathematics and basic understanding of the Matlab programming environment is desirable.

Co-supervisor: Brian Grimes

JOHS-3: Properties of tetraacids and interactions with other indigenous crude oil Components

Tetraacids are highly interfacially active compounds in crude oil which react with divalent cations from water, especially calcium, forming a sticky, gel-like film which accumulates at the oil-water interface, causing expensive shutdown periods. To gain further knowledge of the mechanism and drive forces behind the interfacial precipitation, we wish to study tetraacids with respect to their 1) rheological properties of the gel formed upon reaction and 2) the influence of other crude oil components, *e.g.* monoprotic acids (model and indigenous compounds) and asphaltenes, onto the gellation of Ca^{2+} -TA film. The project is expected to result in highly desired information for the petroleum industry about the structure and rheological properties of naphthenate precipitation, and how to prevent the gellation. The laboratory work will be carried out by using surface/interfacial analysis instrumentation in-house at the Ugelstad Laboratory such as the pendant drop technique, rheometer, Interfacial Shear Rheometer and the Langmuir trough technique. This diploma project will be a part of the *Joint Industrial Program 2* project, with several central oil companies as participants.

Co-supervisors: Erland I. Nordgård/Sebastien Simon

GØ: Professor Gisle Øye

GØ-1: Adsorption-desorption studies related to Enhanced oil recovery by Low Salinity terflooding

Injection of low salinity water into oil reservoirs is a method to increase the oil recovery from oil fields. The interactions between reservoir surfaces, crude oil and water are essential in this method. The project will focus on adsorption/desorption studies using the Quartz Crystal Microbalance technique, in order to understand how composition of oil, water and solid will affect the amount of oil recovered in the process. Other characterisation methods will also be included.

The project will be carried out in collaboration with Statoil and Department of Petroleum Engineering and Applied Geophysics (NTNU).

Supervisors: Gisle Øye and Umer Farooq

Reserved for Naveed Asif

GØ-2: Characterisation and rheological properties of gas hydrate model particles

Gas hydrates are crystalline, water based solids that can cause problems during transport of oil, gas and water. The project will focus on characterisation and rheological properties of dispersions containing model gas hydrate particles.

The project will be carried out in collaboration with SINTEF, IFE and industrial companies.

Supervisors: Gisle Øye and Asal Amiri

GØ-3: Preparation and functionalisation of nanostructured alumina

The project focuses on preparation of porous alumina monoliths functionalised with metallic nanoparticles. Characterisation of the materials will include XRD, gas adsorption and spectroscopic techniques, as well as testing of the materials as catalysts for fine chemicals production.

The project will be carried out in collaboration with SINTEF and Silesian University of Technology (Poland)

Supervisors: Gisle Øye and Bartłomiej Gawel

WRG: *Førsteamanuensis Wilhelm R. Glomm*

WRG-1: Hydrogels with tailored properties

Background: Hydrogels are crosslinked networks of water-soluble polymers. Due to the crosslinks they do not dissolve in water. Instead they swell in aqueous media to increase their weight with several hundred percent. Of special interest are hydrogels with pre-determined mesh size and/or revealing a stimuli-responsive behaviour and degradation, as well as the possibility of functionalisation / ligand immobilization throughout the network. Hydrogels find applications in many fields including medical applications, “smart” materials and controlled release.

In this project, the synthesis and properties of tailored organic/inorganic “hybrid gels” will be investigated. The hybrid gels under investigation consist of different water soluble polymers which are crosslinked by silica domains. The type of polymer used determines the chemical properties of the gel. The amount of silica crosslinks on the other hand determines the pore size and the mechanical properties of the gel.

Project: The project is a co-operation between the Department of Chemical Engineering, NTNU (IKP) and Sintef Materials and Chemistry. It involves both synthesis of different hydrogels and their characterization. We estimate that the project may be suitable for either one or two students.

Contact persons: *Wilhelm Glomm, IKP, e-mail: glomm@nt.ntnu.no, Phone: 73 59 41 58*

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WRG-2: Corrosive sulfur in transformer oils

Electric transformers are key elements of the infrastructure providing electricity for domestic and industrial use. Corrosion of the copper windings and undesired deposition of copper-oxygen-sulfur species leading to short circuits is a growing problem in this industry, and the quality of the transformer oil used as insulator and cooling agent in the transformers is believed to be important. Additives to the oil (referred to as metal passivators) are used in order to prevent failure, but little is known about the mechanism of these passivators. It is however believed that they adsorb on the metal surface and block the interaction with corrosive species in the oil. An important question is related to when the passivator might be added to the system and still act as an effective protection towards deposition of copper-oxygen-sulfur species. Hence, if the corrosion has already started, will the added passivator protect the affected area? In this project we propose a model study, where the interaction between the copper metal and the passivator is studied. This requires very sensitive measurements, so the purpose of the project proposed here is to investigate if the QCM-technique (Quartz Crystal microbalance) is a suitable and sufficiently sensitive tool in order to detect the interaction between the copper metal and the passivator in the oil. The proposal is part of a collaboration with SINTEF Energy Research, and is linked with a large project funded by the Research council and Norwegian and international industry. The project is proposed in collaboration between the Ugelstad laboratory (QCM method) and the Catalysis group (transformer oil project).

Supervisors: *Wilhelm Glomm, Edd A. Blekkan, Ingvild Tronstad, Marit-Helen G. Ese (SINTEF Energiforskning).*

Reserved for Marius Roel

Prosess-systemteknikk/Process Systems Engineering

SiS: ***Professor Sigurd Skogestad***

SIS-1: Self-optimizing Control of a Methanol Process

Methanol can be produced from different sources like natural gas, coal, biomass and petroleum. A methanol plant has 3 main parts (i) production of synthesis gas, (ii) methanol reactor (iii) purification. Various technologies for producing synthesis gas and different types of methanol reactor, catalyst and kinetics are available in literature. In particular, Auto-Thermal Reforming (ATR) is claimed to be the best option to supply synthesis gas for large methanol plant capacities.

In this work, we study in a detail a process based on ATR for synthesis gas production and a fixed bed methanol reactor (Lurgi technology). The well-known Graaf kinetics is used for the methanol reactor; the remaining reactions are simulated assuming thermodynamic equilibrium.

The UniSim process simulator is used to simulate and optimize a methanol plant with a capacity of around 5000 tons/day, which is a current large industrial scale capacity.

The process includes heat integration, high-pressure CO₂ removal, recycles and purge. Important process parameters, which are subject to optimization, include feed rates of water and oxygen relative to methane, reactor temperatures, pressures and recycle flows.

In addition to determine the process and equipment design, optimization in two modes (I- feed is given and II-feed is also a degree of freedom) is used to find optimal operation (control) policies where an important issue is: What should we control? To answer this in a systematic manner we first need to define operational objective (which in this case is to maximize the profit of the plant) and operational constraints (such as maximum and minimum temperatures and minimum stream to carbon ratios).

Next, we optimize the operation for various disturbances (such as feed flowrate, feed composition, pressure and temperature, constraint values, etc.). The first thing we need to control is the active constraints, for example, the minimum amount of steam. Next, we look for “self-optimizing variables”, which are controlled variables which indirectly give close-to-optimal operation when held at constant setpoints, in spite of changes in the disturbances variables.

Co-supervisor: PhD student, Mehdi Panahi

Reserved Theophilus Arthur

SIS-2: Dynamic simulation of liquefaction process for natural gas

LNG (Liquefied natural gas) is still a growing business, both in Norway and abroad. Liquefied natural gas (LNG) is produced by cooling natural gas in several stages to about -162C so that it can be stored as liquid as atmospheric conditions. The volume is then reduced by a factor of about 600. The process is energy and capatial intensive and many alternative designs have been proposed. One is the Mixed Fluid Cascade (MFC) used by Statoil at Hammerfest, but there are also simpler processes. We want to optimize the operation of such plants, and one approach is to make dynamic models and see how they respond to different disturbances and different choices of controlled variables with the goal of identifying “self-optimizing” controlled variables.

As steady-state optimization of this kind of process has showed to be difficult, the dynamic approach is interesting. By building the model, the students can develop understanding for dynamic modelling, then simple feedback control can be implemented in single-input single-output controllers and optimization can be done by changing the setpoints of the unconstrained controlled variables. The basis for the project is an existing model of the process in Hysys/Unisim , MATLAB or gPROMS. This project will thus cover the following topics:

- Dynamic modelling
- Process control
- Optimization

Co-supervisor: Magnus G. Jacobsen

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

We have worked for many years on new integrated distillation sequences, including Petlyuk distillation and the Kaibel column. We have buildt an experimental column which is operated experimentally during 2009-2010.

In this project, the focus will be on design, whereas two other projects will focus on operation and control.

More specifically, the goal of this project is to look for the optimized thermally coupled distillation sequences for multi-component separations. A rigorous model is developed in UNISIM and MATLAB or GAMS will be used for the optimization. So, the capabilities of both softwares are used at the same time. Different alternatives are simulated in UNISIM and then the best option should be selected considering the energy savings through a proper optimization of the interconnecting streams.

Co-supervisor: Maryam Ghardran/Ivar J. Halvorsen (SINTEF)

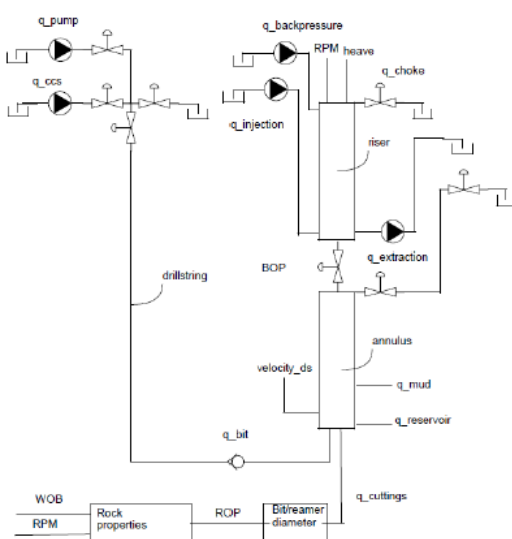
SIS-4: Automated drilling

The drilling process is controlled by machines mainly operated manually by drillers. The task is to drill fast and safe while keeping within a set of boundaries and handle upsets. It is a challenge to coordinate the hardware tools involved in drilling (top drive, pumps, chokes, etc). There is a great potential by increased automatization and optimization. Statoil alone drills for appr 50 MRD NOK/year and the drilling industry operates with a 20-25% non-productive time in average. The main objective is to maximize the drilling efficiency, e.g. represented by the rate of penetration (ROP) and time spent to perform standard operations such as connections. Other parameters are drill bit wear, wellbore pressure, cuttings removal, drill string

torque load, pump flow rates, and choke opening (MPD). Advanced PDE models have been developed mainly for planning and these have also been used in real time during drilling in some operations.

1) The drilling process: A plantwide control approach for optimization

The task is to study the drilling process and to make a *simple* model for control. A starting point can be the pressure-model (Kaasa-model). A task is to make a simple model for rate of penetration (ROP). Both the Kaasa-model and the model for ROP should be used to do a systematic analysis to find the controlled variables and manipulated variables. Further, the best way to pair the variables.



**Co-supervisor: John-Morten Godhavn (Statoil),
Esmaeil Jahanshahi**

In cooperation with Statoil and Siemens

2) Simulation and control of the drilling process: Feedback or feedforward?

A high fidelity Matlab model of a well is available from IRIS. In this project we want to study the application of such a model for control or if it is sufficient to use feedback control from measurements. Controller analysis of poles, zeros, time constants, deadtimes.

Supervisor: Sigurd Skogestad, Co-supervisor: John-Morten Godhavn (Statoil), Esmail Jahanshahi
In cooperation with Statoil and Siemens

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

This project is motivated problems with riser slugs in offshore fields in the North Sea. The objective is two-fold

1. Compare and analyze alternative simplified model of the process.
2. Tune the simple model based on experimental data on our mini-rig so that it represents the actual behavior
3. Discuss the possibility for avoiding the slug flow, for example, by use of active control.

It is also possible to do experiments on a small-scale rig.

Co-supervisors: Weiwei Qiu (postdoc), Esmail Jahanshahi (PhD student) and Professor Ole Jørgen Nydal

SIS-6: Model reduction for fast MPC

The goal is to make a framework for evaluation of reduced models when the reduced model is to be used in closed-loop model predictive control (MPC). The tool we use is bilevel programming, see [1].

The student should have an interest for Matlab and programming in general.

References

[1] Henrik Manum, Colin N. Jones, Johan Löfberg, Manfred Morari, and Sigurd Skogestad: "Bilevel programming for analysis of low-complexity control of linear systems with constraints", Conference on Decision and Control, Shanghai, 2009.

Co-supervisor: Henrik Manum

SIS-7: Dynamic simulation of alternative control strategies

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

Links to descriptions of the software:

[http://hpsweb.honeywell.com/Cultures/en-](http://hpsweb.honeywell.com/Cultures/en-US/Products/ControlApplications/AdvancedControlOptimization/ProfitController/default.htm)

[US/Products/ControlApplications/AdvancedControlOptimization/ProfitController/default.htm](http://hpsweb.honeywell.com/Cultures/en-US/Products/ControlApplications/AdvancedControlOptimization/ProfitController/default.htm)

<http://hpsweb.honeywell.com/Cultures/en-US/Products/ControlApplications/Simulation/default.htm>”

Co-supervisor: PhD student Ramprasad Yelchuru

SIS-8: Self-optimizing control of batch processes

Based on a dynamic model (in Matlab or gProms) of a batch reactor or batch distillation column, the task is to test out alternative self-optimizing control strategies. The objective is to minimize the batch time

Co-supervisor: PhD student Håkon Dahl-Olsen

SIS-9: Modelling and Control of District heating systems

In Trondheim there is a district heating network for hot water based on the Tiller incineration plant for burning waste, and in Oslo there are similar plants. It is possible to save energy by improving the operation and control of such systems. This will be a continuation of a successful ongoing project in cooperation with Helge Mordt at Prediktor (Fredrikstad) who has been working with the Oslo plant.

In practice most district heating systems are controlled by very simple decentralized control. Many decisions are made based on experience and best practice. The scope of this work is to apply a model based systematic approach to the control of a district system.

The master project consists of following parts

- Literature study
- Modelling (we have a model, but it has to be checked and possibly modified)
- Optimizing to find a good nominal operation point
- Designing a self-optimizing control structure or alternatively a MPC controller

Co-supervisor: PhD student Johannes Jäschke

SIS-10: Simple rules for retuning of control loops

Most PID tuning rules, for example the SIMC tuning rules, assume that one has available a simple process model obtained from open-loop experiments. The objective is to extend the tuning rules to the closed-loop case where a controller is already in operation. The task is to identify if control can be improved by retuning and propose rules for the retuning.

Co-supervisor: Mohammad Samsuzzoha

HP Professor Heinz Preisig

HP-1: On time scaling in chemical processes

Project description

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-2: Computer-aided modelling

Project description

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

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

HP-3: Control lab rejuvenation

Project description

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

The control lab shall be updated and augmented with a couple of experiments. Initial plans have been developed. We invite to help thinking about possible, interesting processes and their realisation.

We have now rebuild the distillation columns but should further work on them. Objective is to move the heat exchangers down and make them more look and operate like its industrial counter parts. Besides other issues I am thinking of implementing an original solution for on-line flow measurement and control of the reflux pump.

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

HP-4: Felles Lab Experiments

Project description

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

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

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

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

HP-5: 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-6: Automatic Safety and Hazard Analysis

Project description

Safety and hazard analysis are done mostly in a systematic way, but based on mental models of the process. We would like to change this and use a model-based approach. Starting from a model of a continuous process, we have software that computes the possible things that may happen if the environment changes or faults occur.

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

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

HP-7: Simple Thermo Server

Project description

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

Supervisors: Heinz A Preisig, Tore Haug-Warberg

TH-W: Førsteamanuensis Tore Haug-Warberg

TH-W-1: Thermodynamics of LNG plants: Thermodynamics of LNG plants using the GERG equation of state

Background:

Equations of state based on Helmholtz energy are increasingly used for calculations (modelling and simulation) of industrial processes. The motivation for progress in this field is that a good numerical model of the mass and energy balances of the plant is very useful in all stages of plant design, operation, and safety analysis. The prime concern of such models are the mass and energy (heat) balances, but also the volumetric (flow) properties are of great interest as they allow for a combined fluid flow and thermodynamic calculation of heat exchangers, reactors, valves, pipes, etc. The aim of this project is to implement, test and make use of the “The GERG-2004 Wide-Range Equation of State for Natural Gases and Other Mixtures” which is the result of a large European research program on the accurate description of LNG mixtures for international energy trade (E.ON Ruhrgas, Germany; Enagás, Spain; Gasunie, The Netherlands; Gaz de France, France; Snam Rete Gas, Italy; and Statoil, Norway).

Goal:

Implement (with assistance of the supervisors) the GERG equation of state and make appropriate (numerical) tests to verify thermodynamic consistency. Validate the implementation using experimental densities and vapor-liquid equilibria, possibly also speed of sound and enthalpies of vaporization. The student shall finally make use of the GERG equation to simulate a small yet realistic LNG plant in order to get some experience with the numerical properties of this equation. The student must be motivated to read up a little on equation of state theory and thermodynamic phase equilibrium in general.

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.

Supervisors: Tore Haug-Warberg/Heinz A Preisig.

Reserved

TH-W-2: **Process simulation using YASIM. Further development and use of the Yara Process Simulator (YASIM).**

Background:

In big chemical industries like Yara (one of 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 is used to administrate the requests from an Excel 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. A prototype Excel client is under development at Yara, while simple text based clients are omnipresent using TELNET over TCP/IP.

Goal:

1) Implement, in co-operation with Yara, simple unit operations like heat exchangers, small distillation columns, valves, etc. using the Yasim query language. 2) Look at strategies for solving small flowsheets with recycle streams, or 3) look at possibilities for doing dynamic simulation of the same. Small in this context means 5-20 unit operations.

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. Are Mjaavatten

Reserved

NS-B: Førsteamanuensis Nadi Skjøndal-Bar

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



Systems biology is a fascinating field that aims at system-level understanding of biological systems. It was only recently that system-level analysis can be grounded on discoveries at molecular-level. What does it mean to understand at "system level"? Unlike molecular biology which focus on molecules, such as sequence of nucleotide acids and proteins, systems biology focus on systems that are composed of molecular components. Although systems are composed of matters, the essence of system lies in dynamics and it cannot be described merely by enumerating components of the system. Within this context, (1) understanding of structure of the system, such as gene regulatory and biochemical networks, as well as physical structures,

(2) understanding of dynamics of the system as well as construction of theory/model with powerful prediction capability and (3) understanding of control methods of the system, are key milestones to judge how much we understand the system. There are numbers of exciting and profound issues that are actively investigated, such as robustness of biological systems, network structures and dynamics, and applications to drug discovery. Systems biology is in its infancy, but this is the area that has to be explored and the area that we believe to be the main stream in biological sciences in this century.

It was found in the last decade that gene expression is mainly effected by the initiation process.

Eukaryotic initiation factors (eIF-) 2 are molecules exist in almost every cell of our body. They were found to regulate gene expression, by enabling a ribosome structure to bind to a pre-initiation complex. This process is complex and involves many different regulating components. A simplified

model of the eIF-2 regulation process was developed using a non-linear state space framework (see Bar and Morris, 2007). Simulations and analysis of the reduced model led to several conclusions about the effect of a few principle factors in the eIF-2 initiation process, consistent with recent experiments in yeasts.

The aim of the Project includes: (1) a background study of the eIF-2 regulation process, (2) Exploration of robustness of the model to noise (disturbances) and (3) sensitivity analysis of the model. It is highly desired that the project will be integrated with the Master thesis, (Diplomoppgave), spring 2010. Pre-knowledge in biology, genetics, and molecular biology is an advantage, but is not essential for the success of the project/Diplom. The candidate can easily establish a career in Systems Biology as modeler, researcher and systems engineer both in the industry (for instance in medical companies) and particularly in the academy (PhD programs all over the world).

Further details about the project and diplom opportunities can be acquired at 735-94124 or email nadi.bar@ntnu.no

Further reading:

Systems biology:

H. Kitano, Systems Biology: a brief overview, Science, 295:1662-1664, 2002

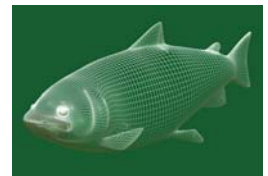
H. Kitano, Computational Systems Biology, Nature, 420:206-210, 2002

Control of Protein Expression:

N. Skjøndal-Bar and D. Morris: Dynamic model of the process of protein synthesis in Eukaryotic cells, B. math.Bio, 69:361-393, 2007

Supervisor: Nadi Skjøndal-Bar

NS-B-2: Systems Biology - Modelling Feed intake and appetite of fish



Do you like solving mysteries and riddles? Do you find living systems fascinating? Are you interested to find out how, why, and when we are hungry? A project aiming to solve the mystery of appetite and feed intake in fish is underway, at the Department of Chemical Engineering, Systems Biology (process control group). The question of appetite is crucial since it has the greatest impact on the growth of the organism (in this case fish). The fish prefers certain types of feed based on there composition (protein content, energy and nitrogen levels). for instance, unbalanced feeds elevate the nitrogen levels in the blood, which sends feedback to the enzymes in the stomach and the gut, ultimately affecting appetite.

The aim of the Project includes: (1) Identify the factors that affect the appetite of fish (particularly Atlantic salmon) (2) integrate these factors into a system, creating a qualitative model and (3) develop a quantitative model of the system or parts of it.

It is highly desired that the project will be integrated with the Master thesis (Diplomoppgave), spring 2009. Pre-knowledge in biology is an advantage, but is not essential for the success of the project/Diplom. The candidate can easily establish a career in Systems Biology as modeler, researcher and systems engineer both in the industry (for instance in BioMar AS) and particularly in the academy (PhD programs). The project and thesis have high potential for publications due to the innovative framework.

About systems biology:

Systems biology is a fascinating field that aims at system-level understanding of biological systems. It was only recently that system-level analysis can be grounded on discoveries at molecular-level.

What does it mean to understand at "system level"? Systems biology focus on systems that are composed of molecular components. Although systems are composed of matters, the essence of system lies in dynamics and it cannot be described merely by enumerating components of the system. Within this context, (1) understanding of structure of the system as well as physical structures, (2) understanding of dynamics of the system as well as construction of theory/model with powerful prediction capability and (3) understanding of control methods of the system, are key milestones to judge how much we understand the system.

There are numbers of exciting and profound issues that are actively investigated, such as robustness of biological systems, network structures and dynamics, and applications to drug discovery. Systems biology is in its infancy, but this is the area that has to be explored and the area that we believe to be the main stream in biological sciences in this century.

Further details about the project and diplom opportunities can be acquired at 735-94124 or email nadi.bar@ntnu.no

Further reading:

Systems biology:

H. Kitano, Systems Biology: a brief overview, Science, 295:1662-1664, 2002

H. Kitano, Computational Systems Biology, Nature, 420:206-210, 2002

Dynamic Model of fish growth:

N. S. Bar, T. sigholt, K. D. Shearer and Å. Krogdahl: A dynamic model of nutrient pathways, growth and body composition in fish, Can. J. Fish. Aquat. Sci. 64(12):1669-1682, 2007.

Supervisor: Nadi Skjøndal-Bar

Reserved Martin Buus Jensen

Miljø- og reaktorteknologi/Environmental Engineering and Reactor Technology Group

Reaktorteknologi

HAJ *Professor Hugo Atle Jakobsen*

HAJ-1: Numerical investigation of integrated reactor-separator designs for pre-combustion with CO₂ 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 CO₂ 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 CO₂ and desorption of CO₂ from the adsorbents. To optimize the reactor performance with CO₂ capture, we may consider the possibility to reduce the operating temperature, reduce the reactor volume, lower pressure, intensify heat integration and to reduce emissions fluxes compared to the conventional steam methane reformer process. The first part of the work consists in deriving suitable models for the different reactor types. Then, the models should be implemented in matlab and solved with a suitable numerical method.

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

Supervisor: Hugo A. Jakobsen

HAJ-2: Numerical analysis of multicomponent mass diffusion in catalyst pellets for combustion with and without CO₂ capture.

A consistent model for multicomponent mass diffusion is derived and we want to perform model validation. Traditionally 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 formulation.

For this purpose we may use the catalyst pellets for steam methane reforming (SMR) and the pellets for sorption enhanced steam methane 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 orthogonal collocation.

Supervisors: Hugo A. Jakobsen and Magne Hillestad

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

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

In this work we intend to outline the possible reactor designs and to model and simulate a few of the possible reactors for these processes. To optimize the reactor performance with CO₂ capture, we may consider the possibility to reduce the operating temperature, reduce the reactor volume, lower pressure, intensify heat integration and to reduce emissions fluxes compared to the conventional processes. The first part of the work consists in a literature review to find physical data, transport coefficients, reaction equilibrium and kinetics models, and as a second part of the work suitable models for the different reactor types must be formulated. Then, finally, a few (at least one) models should be implemented in matlab and solved with a suitable numerical method.

It is possible to split the project into two parts so that one student may study the CLC process and a second student investigate the CLR process operated within fluidized bed reactors.

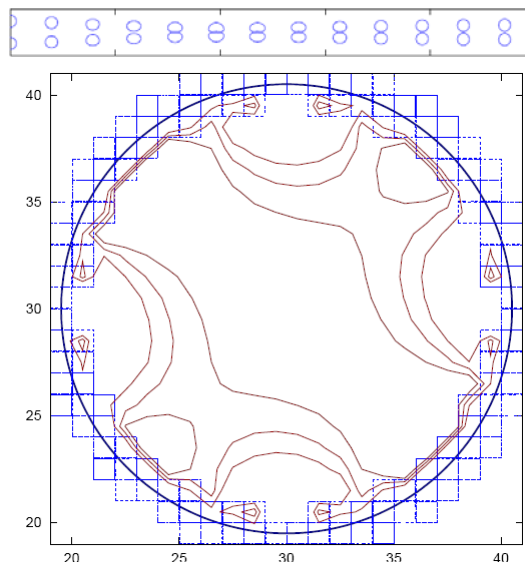
Supervisors: *Hugo A. Jakobsen, Magne Hillestad and NN from Catalysis group*

HS: Professor Hallvard F. Svendsen

HS-1: Multiscale droplet study at different pressures.

Droplets are present everywhere in nature, from rain to mist and in engineering, from gas processes to combustion chambers.

The proposed work is part of a four year project, HiPGLS, proposed “to enhance the understanding and modelling capability of the phenomena governing the separation of liquids from gases at high pressures to such an extent that vendors are able to design and supply compact separators and scrubbers”. The project is integrated by oil companies such as Statoil, Norsk Hydro, Conoco-Phillips, ExxonMobil, and Shell, together with vendors.



The candidate will use an in-house developed code for running droplet simulations. The outputs of these simulations are droplet videos and Matlab files containing the pressure and velocities. The candidate will use her/his knowledge to select the conditions more relevant for the industrial application and interpret the output.

Requirements for the candidate

- Basic Matlab (required)
- Transport Phenomena course (preferred)

Supervisor: *Hallvard F. Svendsen, co-supervisor: Pablo Dupuy*

HS-2: CO₂ absorpsjon: Likevekt- og kinetikk målinger.

For validation of equilibrium and kinetic models for CO₂ absorption, a large range of good experimental data are needed. Together with SINTEF Material and Chemistry we operate many different apparatuses for measuring CO₂-equilibrium for different temperatures and pressures, for kinetics, CO₂ solubility, VLE in unloaded systems and for thermal data. Several PhD candidates work on this and this(ese) diploma task(s) will be performed in collaboration with a PhD candidate.

The work we are doing is in collaboration with Norwegian industry and also leading European laboratories in EU projects. There is flexibility in choice of task, but all task will be a combination of experimental work and modelling. All apparatuses are operative.

Supervisors: *Hallvard F. Svendsen, PhD students and SINTEF personnel.*

HS-3: CO₂ capture from Al-production.

This task is reserved for Renate G. Ringstad

Supervisors: *Hallvard F. Svendsen and Ardi Hartono*

HS-4: CO₂ Capture from power plant exhaust gases

This task is reserved for Shahla Gondal

Supervisors: *Hallvard F. Svendsen and Ardi Hartono*

HS-5: Vapour-Liquid Equilibrium data for acidified NH₃-H₂O-amine systems.

This task is reserved for Stine Roset

Oppgaven utføres delvis i Oslo hos Aker Clean Carbon.

Supervisors: *Hallvard F. Svendsen and Otto Morten Bade (ACC)*

HS-3: High-Pressure Droplet Experiments

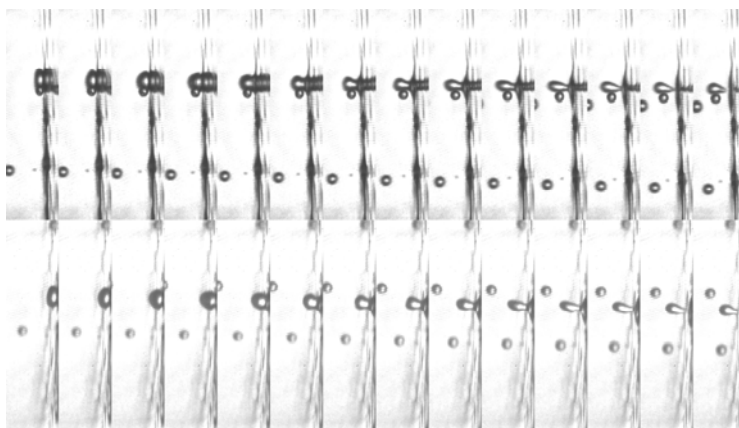
Droplets are present everywhere in nature, from rain to mist and in engineering, from gas processes to combustion chambers.

The proposed work is part of a four year project, HiPGLS, proposed “to enhance the understanding and modelling capability of the phenomena governing the separation of liquids from gases at high pressures to such an extent that vendors are able to design and supply compact separators and scrubbers”. The project is integrated by oil companies such as Statoil, Norsk Hydro, Conoco- Phillips, ExxonMobil, and Shell, together with vendors

The interaction between a droplet and a wall or liquid film may have many outcomes: total, partial or zero deposition of liquid may occur. These outcomes are directly related to the physical properties of the system and the operational conditions in a unit. The sum of these outcomes also determines the separation efficiency of the equipment.

The objective of the experiments is obtaining experimental data of the outcomes of droplet-wall and droplet liquid film collisions at high pressures.

High speed cameras are used to take sequential pictures of the surroundings of a jet in an atomization process. The candidate will run the experiment and analyze the result by mean of computer assisted tools.

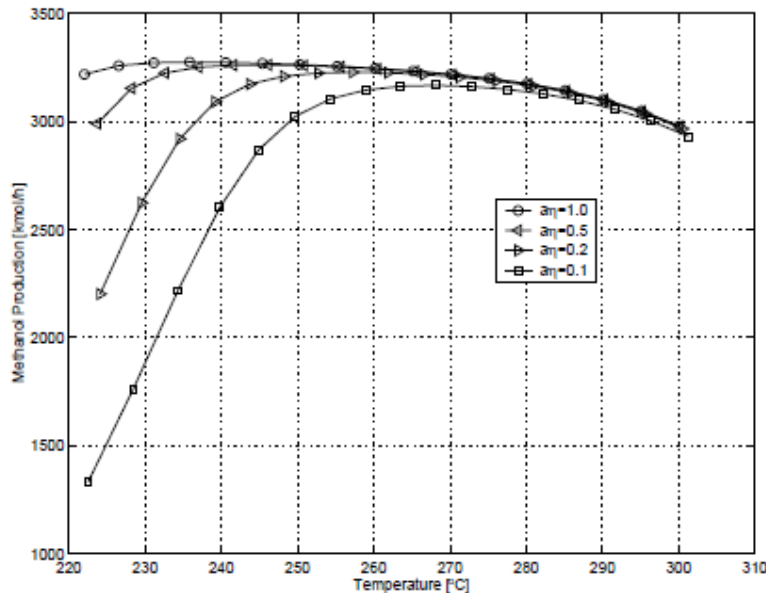


Supervisor: *Hallvard F. Svendsen, co-supervisor: Pablo Dupuy*

MH: Professor Magne Hillestad

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

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



There is 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.

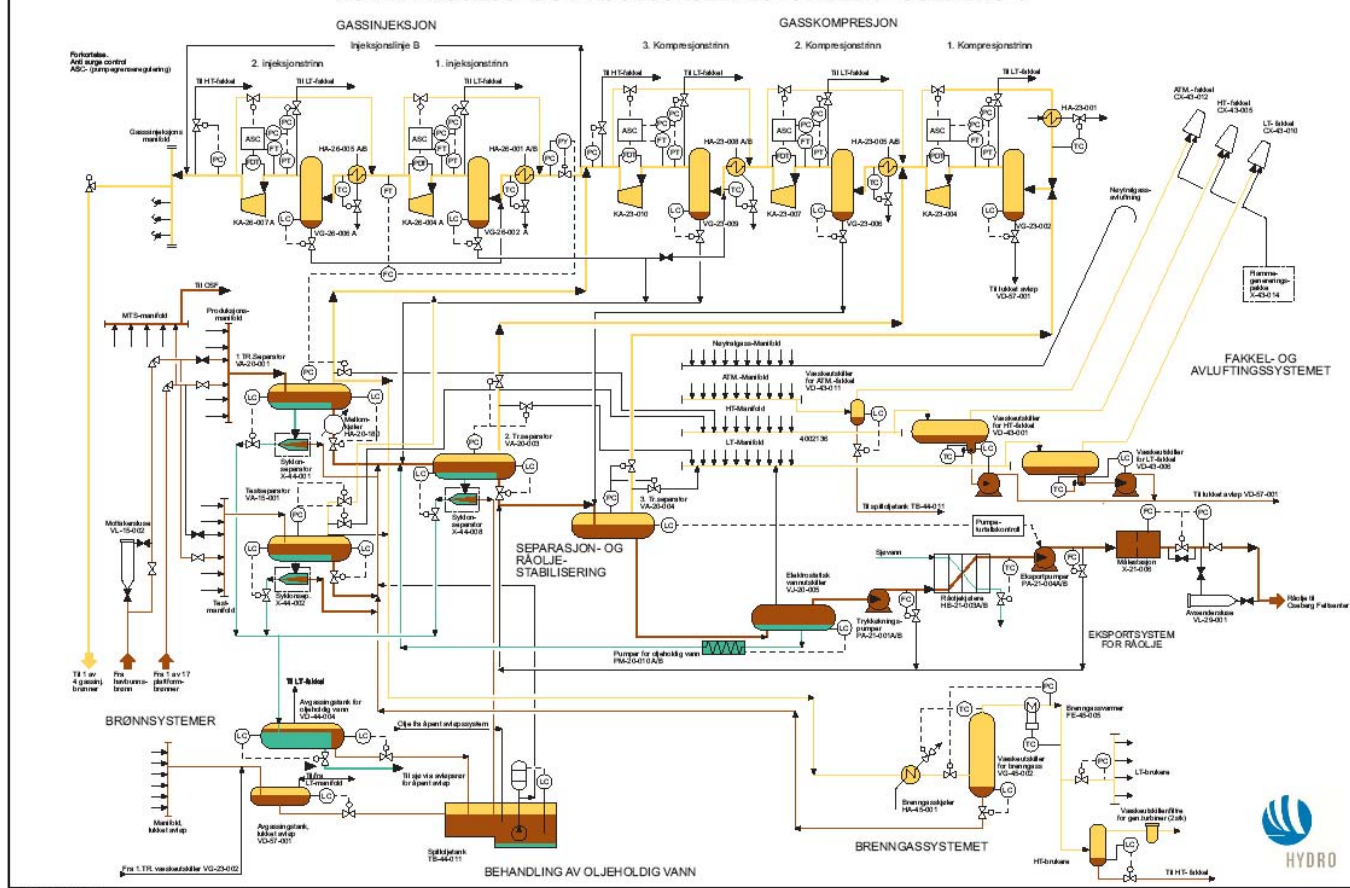
MH-2: Reduce CO₂ and NO_x emissions from offshore oil and gas platforms

This is a project proposed by Statoil research center in Bergen. The main goal is to propose alternatives which can reduce CO₂ and NO_x emissions from offshore platforms. The projects three tasks are:

- Task 1: Identify the CO₂ & NO_x reduction alternatives.
- Task 2: A feasibility study for the integration of wind power to an oil/gas platform.
- Task 3: Develop a general methodology to evaluate the energy effectiveness at offshore platforms.

The focus will be on task 3 applied on the Oseberg C platform in this project.

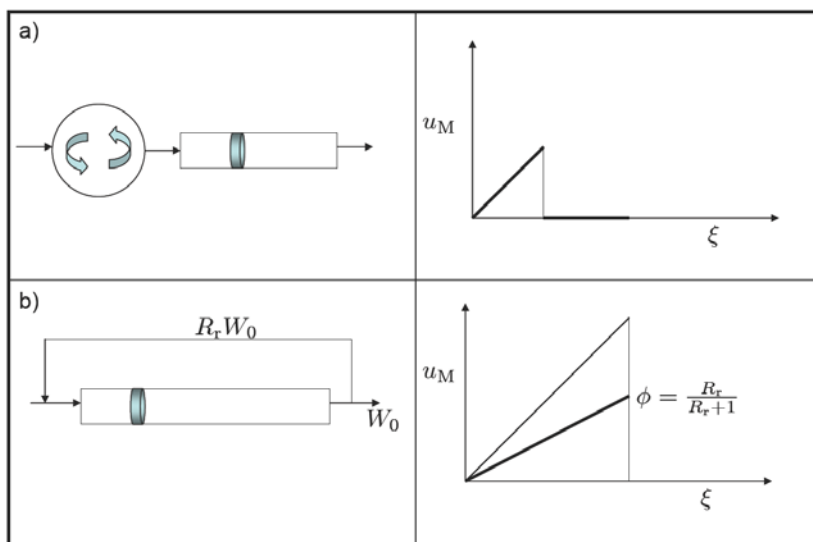
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Co-adviser: Wei He, Statoil Research center Bergen

MH-3: Systematic Staging in Chemical Reactor Design

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



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

units. A kinetic model of the gas phase methanol synthesis is used as an example. By applying the method on the model, a staged reactor design with less heat transfer area and higher production is possible. The method is to be applied on a known system where the kinetics and other phenomena are described. The model will be programmed in Matlab.

MH-4: 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-5: Modelling and optimization of a Gas-to-Liquid plant

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

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

The optimization phase deals with:

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

Co-advisor: Ahmad Rafiee

MH-6: Energy considerations around an amine CO₂ capture plant

Adding a CO₂ capture plant to a power plant will introduce a penalty up to 30%. A post combustion CO₂ capture plant will consist of an absorption column, a stripper, heat exchangers, a blower, pumps, CO₂ 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 CO₂ 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 capturing plant can be modelled in UniSim, Hysys or Aspen plus.

Co-advisor: Mehdi Karimi and Karl Anders Hoff (Sintef)

M-BH-1: Hollow fiber membranes for CO₂ capture

The membrane separation process presents a unique advantage among the other separation process because of low energy consumption and lack of additional chemicals. Processing large volume of gases such as flue gas requires a large membrane area with a minimal foot print. Hollow fibre membrane geometry (Fig.1 a) represents optimum solution due to the high ratio of membrane area per volume. The project will be focused on preparing porous polysulfone hollow fibers by phase inversion using a spinning machine (Fig.1b). Different parameters will be optimised in order to obtain hollow fibers with a precisely controlled geometry and pore size: polymeric solution concentration, spinning speed, additives, coagulation bath, etc.

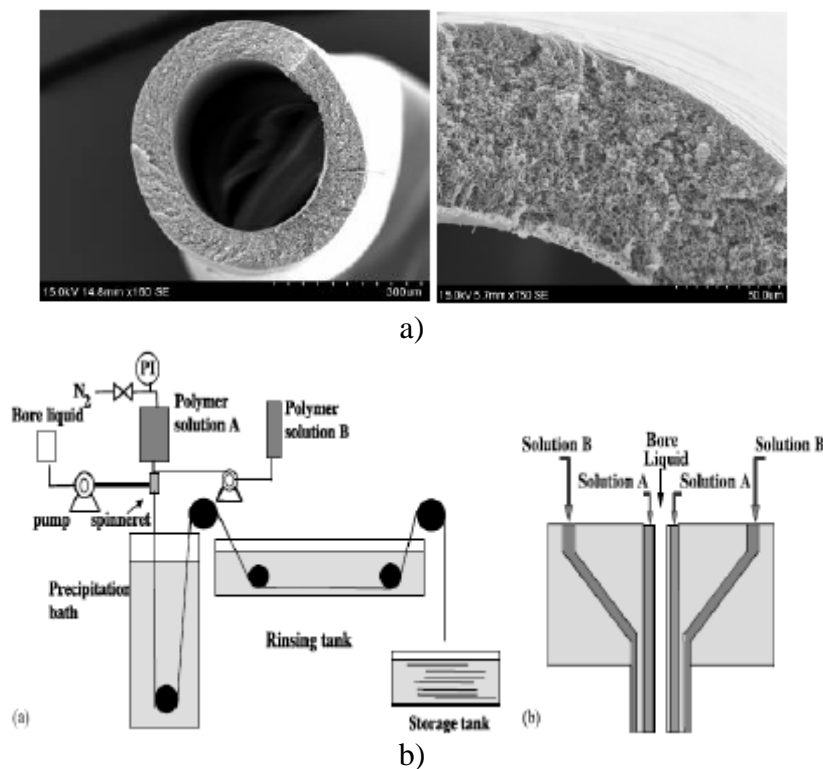


Fig.1 a) Hollow fiber membrane and b) spinning setup

The assignment requires a literature study and practical experiments. The literature study will be focused on optimizing the spinning procedure. The hollow fibers will be investigated by scanning electron microscopy, contact angle, gas permeation and porometry (pore size measurement and pore size distribution).

The hollow fibres will be coated with a dense selective PVAm layer, packed in modules and membrane separation properties will be tested for different gas mixtures such as CO₂/N₂, CO₂/CH₄.

Modules design will be optimized for two coating procedures (inside and outside) and for maximizing the membrane area/module volume ratio. The separation properties will be investigated under different experimental conditions: pressure, temperature, gas flow patterns and relative humidity.

The work will be performed in connection to the large European project, NanoGloWa (Nanomaterials against Global Warming)

Co-supervisor: Dr. Marius Sandru

M-BH-2: Improving durability of the FSC (fixed-site carrier) membranes for CO₂ separation by protective coating

Not even referring to the many recent reports by the experts, the role of CO₂ in the global climate change is now well known and the capture of CO₂ is one of the most popular but very urgent issues to be solved in our generation.

Excellent FSC membranes for CO₂ capture are under active development in MEMFO group (IKP, NTNU). Now the development of these membranes is shifting to pilot scale and commercial test stages where the membranes will meet real gases.

In real gases such as flue gas from power plant or natural gas from gas field, there are many contaminants which might deteriorate the membrane performance of CO₂ separation while the major components are N₂ & CO₂ in flue gas and CH₄ & CO₂ in natural gas.

The major contaminants are SO₂ (or possibly in acidic water vapour form) & NO_x in flue gas and H₂S & higher hydrocarbons & possibly some anti-freezing additives in natural gas.

To protect the FSC membranes from these potential contaminants, one of the well-known methods to be exploited is the use of protective coating of the membrane surface.

The possible candidate materials for coating are Nafion (sulfonated tetrafluoroethylene based fluoropolymer-copolymer), PEEK (polyether ether ketone) and PDMS (polydimethylsiloxane).

In this project;

1) The candidate coating materials mentioned above will be prepared in some suitable solution form (concentration, solvent, etc.) after chemical modifications if necessary.

For example, PEEK may be aminated or sulfonated in order to be more compatible with the surface of the FSC membranes.

2) The FSC membranes will be prepared in pilot scale, but the membranes will be cut out to smaller pieces and coated with some series of the (modified) material solutions. The compatibility (good uniform film forming without a breakage or a defect) of each solution with the sample will be carefully checked to find a best condition for preparing the coating solution of each candidate material.

3) The performance of the coated membranes will be tested with permeation set-up and be compared to that of the non-coated membranes.

4) The coated membranes will be exposed to contaminant gases and then the performance change will be checked and compared.

5) The physical or chemical changes of the membranes before and after the exposure to contaminants will be investigated by FT-IR as well as SEM.

Co-supervisor: Dr. Taek-Joong Kim

M-BH-3 – 4: The effect of contaminants in flue gas and natural gas streams on CO₂ capture performance of FSC (fixed-site carrier) membranes (Contaminants on Natural Gas Membranes)

Use of membrane for CO₂ capture has begun to attract a strong attention thanks to crucial advantages such as low energy consumption and environmentally friendly process compared to the conventional amine solvent absorption technique where chemicals that are potentially hazardous are used.

Two types of FSC membrane for CO₂ capture have been developed in MEMFO group (IKP, NTNU) for several years. One is a PVAm (polyvinylamine) based membrane and the other one is a blend membrane of PVAm and PVA (polyvinylalcohol).

They have different chemical & physical properties so that PVAm membrane is expected to be used for flue gas CO₂ capture and the blend membrane for natural gas sweetening.

In real flue gas and natural gas streams there are several contaminants that would potentially harm the membrane performance. For example, they may be SO₂ & NO_x in flue gas and H₂S & higher hydrocarbons in natural gas.

In this project the effect of those major contaminants will be investigated;

- 1) The membranes will be prepared in pilot scale under different conditions.
- 2) The membranes will be exposed to the contaminants under certain different conditions and then the performance change will be tested using lab.scale membrane performance test set-up and high pressure durability set-up. For some of the sample membranes, the high pressure durability set-up will be used especially for H₂S & higher hydrocarbon contamination study at higher pressure.
- 3) The possible physical or chemical changes of the membranes before and after the exposure to contaminants will be investigated by FT-IR as well as SEM. The FT-IR is expected to enable investigation especially on the possible reaction of SO₂ or NO_x with the membrane materials which might affect the CO₂ transport ability of the membranes if the reaction is identified by this special instrument, FT-IR.

Co-supervisor: Dr. Taek-Joong Kim

Reserved for Camilla Hesstvedt

M-BH-5: Optimization of the CNTs reinforced PVAm/PVA blend membranes

This master thesis will focus on the optimization of the carbon nanotube (CNT) reinforced polyvinylamine/polyvinylalcohol (PVAm/PVA) blend membrane for high pressure applications, such as natural gas sweetening process. CNTs are considered as the nano-filler in making the PVAm/PVA blend based nanocomposite membranes. The functions of the CNTs in this membrane include the reinforcement of the membrane mechanical properties and the improvement of the membrane swelling capacity (and hence CO₂ separation efficiency) at high pressures due to the nano spacer effect of the CNTs.

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

- (1) Selection of commercially available, water dispersible CNTs
- (2) Optimization of the dispersion of selected CNTs in blend solutions
The CNT loading, CNTs dispersion protocol and the concentrations of casting solution will be optimized,
possibly with an orthogonal experimental design.
- (3) Permeation test of the CNT-blend membranes
- (4) Characterizations of the CNT-blend membranes
Further characterizations of the CNTs-blend membranes will be carried out to quantify the improved properties, including mechanical strength, FTIR, XRD, sorption of gases at high pressures.
With results from above listed work, this project may contribute significantly to the commercialization of the FSC membrane in the natural gas sweetening process and further more, to the promotion of the green and energy saving membrane approach in CO₂ capture solutions.

M-BH-6: Optimization of high pressure resistant blend membranes

This master thesis will focus on the optimization of the preparation procedure of a patented polyvinylamine/polyvinylalcohol (PVAm/PVA) blend membrane for natural gas sweetening. The objective of this work is to improve the target membrane to be more resistant at high pressures without the loss of the CO₂ separation efficiency.

The tasks of this thesis work can be specified as follows (only a few selected tasks will be focused on in one MSc thesis – two thesis works may be defined from the list below):

1. Investigation of the effects of the molecular weight of PVAm in the blend membrane
PVAm/PVA blend membrane with the commercially available PVAm of different molecular weight (e.g, PVAm 25,000 from Polyscience Inc. and 50,000 and more from BASF) will be prepared and their respective permeation rates at pressures from 2-15bar be compared. The mechanical properties of these blends will be measured.
2. Optimization of dip-coating procedure
To achieve the precise control of the coating layer thickness, the effect of the viscosity, concentration of casting solutions and the coating layers on the coating thickness will be optimized, possible with an orthogonal experimental design.
3. Cross-linking of the blend membrane
Heat cross-linking of the blend with various temperatures and duration for blend of different PVAm molecular weight will be optimized, along with the chemical cross-linking of the blend with 2-3 different cross-linking agents, and the effects of different cross-linking methods on high pressure resistance and permeation will be evaluated.
4. Characterization of the blend membranes
Further characterizations of the optimized blend membrane will be carried out to quantify the improved properties, including mechanical strength, FTIR, XRD, sorption of gases at high pressures.
5. Investigation of the effects of the molecular weight of PVAm in the blend membrane
PVAm/PVA blend membrane with the commercially available PVAm of different molecular weight (e.g, PVAm 25,000 from Polyscience Inc. and 50,000 and more from BASF) will be prepared and their respective permeation rates at pressures from 2-15bar be compared. The mechanical properties of these blends will be measured.
6. Optimization of dip-coating procedure
To achieve the precise control of the coating layer thickness, the effect of the viscosity, concentration of casting solutions and the coating layers on the coating thickness will be optimized, possible with an orthogonal experimental design.
7. Cross-linking of the blend membrane
Heat cross-linking of the blend with various temperatures and duration for blend of different PVAm molecular weight will be optimized, along with the chemical cross-linking of the blend with 2-3 different cross-linking agents, and the effects of different cross-linking methods on high pressure resistance and permeation will be evaluated.
8. Characterization of the blend membranes
Further characterizations of the optimized blend membrane will be carried out to quantify the improved properties, including mechanical strength, FTIR, XRD, sorption of gases at high pressures.

With results from above listed work, this project may contribute significantly to the commercialization

of the FSC membrane in the natural gas sweetening process and further more, to the promotion of the green and energy saving membrane approach in CO₂ capture solutions.

Co-supervisor: Dr. Liyuan Deng

M-BH-7: Production of carbon hollow fibres for air separation

There are several reasons why air separation may be valuable. For instance, nitrogen can be used as blanketing gas, or the air composition can be tuned for combustion purposes.

It is the scope of this work to cover all steps in making a membrane module that is useful for air separation.

Part A

Polymeric hollow fibres are going to be spun according to an established procedure with a given dope solution. Targets for precursor production include:

- Reducing the cost and time of the fibre post treatment, without having the carbon fibre performance reduced.
- Identify successful drying conditions, including a.o. temperature, stretch and chemicals.

Resulting fibres should be characterized by appearance, dimensional changes, microscopy and morphology analysis.

Co-supervisors: Dr. Jon Arvid Lie and Dr. Arne Lindbråthen (MemfoACT)

Reserved Shamim Haider

Part B

The precursor fibres are then going to be carbonized according to a protocol that results in carbon with high O₂/N₂ separation performance. Cross-sections of the carbonized fibres are going to be characterized by optical microscope and scanning electron microscopy (SEM).

Finally, carbon fibres are going to be measured in permeation rigs at moderate feed pressures, but up to ca 200°C. Important steps include:

- Choice of sealing method, e.g. choice of epoxy
- Single gas tests for screening of fibres (feedback to part A)
- Mixed gas tests for a large module, with different flow configurations

Co-supervisors: Dr. Jon Arvid Lie and Dr. Arne Lindbråthen (MemfoACT)

Reserved Kjetil Skjeldestad

M-BH-8: Influence of pH on salt rejection for osmotic membranes

Background:

At our department we are dealing with sustainable energy technology, e.g. CO₂ capture and renewable energy. One of the more interesting renewable energy sources is the energy of mixing when rivers meet the ocean. This energy may be utilized in so called osmotic power plants. The core technology in such plants is the membrane. Another renewable energy source is biomass that can be fermented into e.g. biobutanol. At DCE we are currently developing membranes for these purposes.

Description:

The membranes we are developing are Thin Film Composite or TFC membranes, prepared by interfacial polymerization. To enhance the water flux through the membrane we are preparing the thin film in a way that we get a hydrophilic surface against the support membrane and the sweet water. Traditional methods give slightly hydrophobic surfaces against the sweet water giving rise to resistance to water flux. On the other hand we end up with a slightly hydrophobic surface against the brine. On the brine side of the membrane we would like to have strong bases or acids in order to create an electric double layer that will hinder the Na⁺ respectively Cl⁻ in entering the membrane, hence increasing the salt rejection. This is a theory we would like to test in the current project by placing organic bases or acids on the surface of a membrane. At lower and higher pH organic bases respectively organic acids will be more dissociated and give rise to stronger electric double layers and increased salt rejection.

Laboratory: The work will be performed in Chemical Building V.

Field of interest (candidate): Knowledge of one of the following subjects will be advantageous: Membrane Science, Polymer Chemistry, Organic Chemistry and/or Environmental Technology.

Co-supervisor: *Senior scientist Tom-Nils Nilsen*

M-BH-8: Influence of gradients in temperature on water flux in osmotic processes

Background:

At our department we are dealing with both theoretical and practical problems. Sometimes it is of great interest to test theoretical ideas in practical experiments. One such issue is how the water flux set up by a concentration and/or a pressure gradient is influenced by temperature gradients over a semi permeable membrane. The results will be crucial in assessing osmotic heat power plants.

Description:

In the current project the problem will be addressed by theoretically calculate the differential pressure over a membrane with different temperatures on each side. In the calculations also the solute concentrations on the two sides of the membrane may be varied. The results will be tested against a steady state experiment, monitoring the solute concentration on the two sides of a hydrophobic micro-porous membrane. The variations in solute concentration will tell us how the various gradients in pressure, concentration and temperature influence the water transport across the membrane. The water will pass the membrane in gas phase and will by evaporation lower the temperature at the hot side, and by condensation increase the temperature on the cold side of the membrane. This will lower the differential temperature, and hence the differential pressure. The temperature will be monitored at the membrane surfaces, and perhaps inside the membrane.

Laboratory: The work will be performed in Chemical Building V.

Field of interest (candidate): Knowledge of one of the following subjects will be advantageous: Thermodynamics, Membrane Science and/or Polymer Chemistry.

Supervisor: *I.aman Tore Haug-Warberg, Co-supervisor: Senior scientist Tom-Nils Nilsen*

Crystallization

J-PA: *Førsteamanuensis Jens-Petter Andreassen*

J-PA-1: Size-enlargement of carbonate particles precipitated during gas production

The off-shore production of natural gas 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 aim of the project is to study the growth rate and agglomeration of particles in the presence of selected agglomerants/flocculants and to evaluate the resulting separation efficiencies by filtration and sedimentation studies.

Supervisor: *Jens-Petter Andreassen/co-supervisor: Ralf Beck*

Reserved

J-PA-2: CO₂-capture in carbonate solutions with simultaneous precipitation

CO₂-capture in carbonate solutions can be an efficient and environmentally benign alternative to the amine based absorption. The absorption capacity increases if the absorption process can allow for simultaneous precipitation of carbonate crystals. Different carbonate solutions will have varying absorption kinetics and regeneration efficiencies. The product of the reaction with CO₂ and ammonium carbonate solutions is ammonium bicarbonate (NH₄HCO₃) that will fall out of the solution as crystals during absorption. Regeneration into pure CO₂ can be obtained at low temperature by the decomposition of these crystals.

An absorber unit has been constructed for this purpose. The aim is to develop the absorption set-up further, to do measurements in different carbonate systems and to compare the results to batch absorption.

Reserved

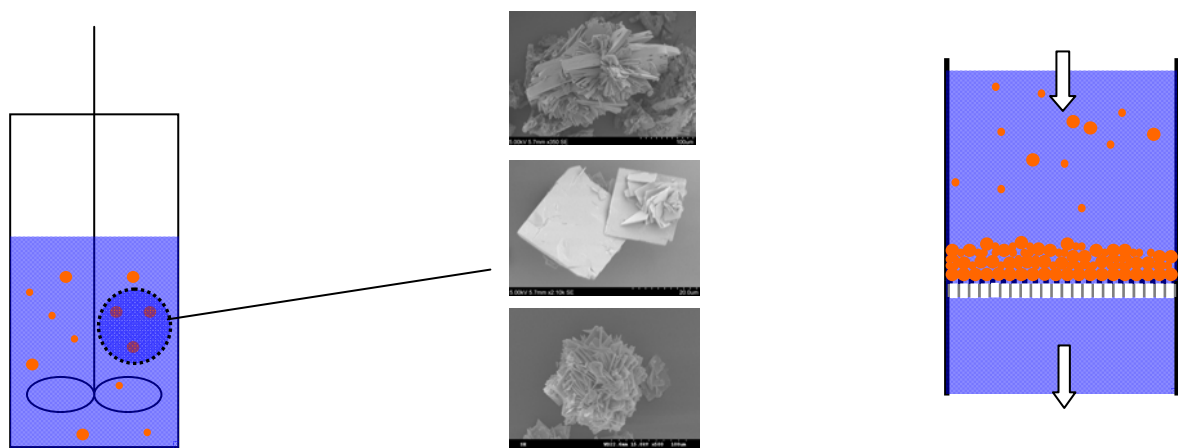
DM-S: *Professor II Dick Malthe-Sørenssen*

DM-S-1: Crystallization of two polymorphs in production of an intermediate in contrast agent production.

GE Healthcare is producing x-ray contrast agents for medical diagnostics. One of the intermediates in the production exhibit two different polymorphs (different crystal structures). One is easily filtered and washed, whereas the other is difficult filter resulting in production stop and reprocessing. The properties of the polymorphs differ with regard to solubility and morphology. It is of great interest to investigate the crystallization of the polymorph with lowest solubility and least filterability since this polymorph will give the best economical result. The investigation will include studies of solubility, polymorph transition, properties of filtration such as cake resistance and porosity. Techniques such as XRD, SEM and filtration techniques will be used.

The aim is to find the most important parameters for controlling the formation of the preferable polymorph in addition to clarify reasons for prolonged filtration time for the polymorph with low filterability.

The starting point will be to find the correlation between crystallization parameters and crystal properties.



Crystallization parameters:

- Temperature T
- Supersaturation S
- Stirring
- Solvent mixture

Crystal properties

- Polymorph
- Form
- Particle size distribution

Filtration

- Porosity
- Cake resistance

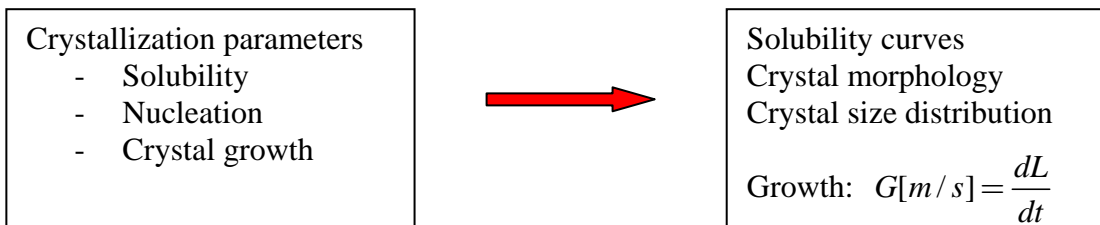
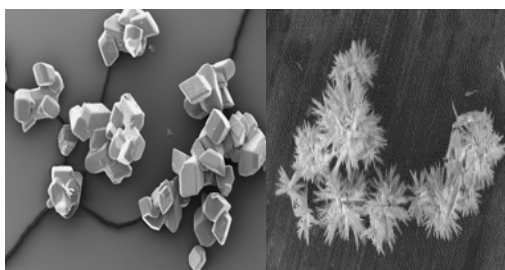
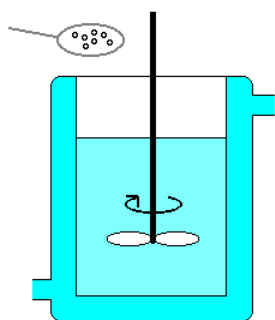
Responsible teacher: Dick Malthe-Sørenssen, supervisor: Jens-Petter Andreassen

DM-S-2: Crystal growth of an aromatic amine, a model substance for production of an x-ray contrast agent.

In the production of contrast agents for medical diagnostics GE Healthcare has an extensive use of crystallization as a separation and purification technique. To control these processes it is important with basic understanding of the parameters influencing the crystallization processes. Some times crystallizations can invoke production stop with loss of capacity and economy.

The aim of the present study is to understand how specific impurities in the production process can inhibit crystallization, nucleation and growth processes and influence the solubility of the active component.

The starting point will be to investigate how inorganic ions influence the solubility, nucleation and crystal growth of a specific system. The formation of different polymorphs will be investigated depending on parameters influencing the nucleation and growth. The aim is to understand the following



Supervisors: Dick Malthe-Sørenssen and Jens Petter Andreassen

Bioraffinering og fiberteknologi/Biorefining and Fibre Technology

SM *Førsteamanuensis Størker Moe*

SM-1: Raffinering av høyutbytte-sulfatmasse

Ved framstilling av høyutbytte-sulfatmasse skjer den endelige defibreringen av vedråstoffet ved raffinering av massen etter kokeren. På grunn av tilfeldige kvalitetsvariasjoner i råstoffet, vil kappatallet i ferdig kokt masse variere, noe som igjen påvirker malebehovet for massen. Ved for høy energiinnsats i raffineringen vil effekten av raffineringen endres fra kun defibrering til en kombinasjon av defibrering og maling, noe som vil påvirke fiberens svellingsegenskaper og dermed massens oppførsel i DD-vask etter raffinøren. Ved Peterson Linerboard i Moss har det blitt utviklet enkle modeller for styring av raffineringen basert på massens kappatall, men disse modellene er ikke gyldige med dagens prosessvariabler.

I oppgaven skal sentrale egenskaper (primært slitindeks, men til en viss grad andre egenskaper som for eksempel malegrad) ved den ferdig silte og vaskete massen kartlegges. Målinger som skal gjennomføres er masseegenskaper som slitstyrke, dreneringsegenskaper, kappatall og KOF (på lab), kappatall (fra prosess-styringssystemet) og energiforbruk under raffineringen (fra prosess-styringssystemet). Med grunnlag i eksisterende modeller skal det undersøkes om man kan finne en korrelasjon mellom kappatall i masse før andrestegsraffinøren, energiinnsats og de målte masseegenskapene. Avhengig av oppnådde resultater kan arbeidet utvides ved å studere virkningen av raffinering på vaskeresultatet.

Opgaven skal utføres ved Peterson Linerboard i Moss.

Faglærer: Førsteamanuensis Størker Moe, medveileder: Professor Øyvind Gregersen, faglig veileder:

Produksjonssjef David Johnson

Opgaven er reservert Pål Eklund

ØWG *Professor Øyvind Weiby Gregersen*

ØWG-1: Colloidal wood resin: characterization, stability, flocculation and interaction with surfaces

Background

Mechanical pulping is an energy-intensive process. In the production of mechanical pulp a large amount of extractives is dispersed into the process water as colloidal droplets and they continue to be a concern to pulp and paper manufactures. Particles of insoluble extractives may later on aggregate and deposit onto paper machine equipment or the formed sheet, thus affecting the runnability of the paper machine as well as the quality of paper.

Deposits are often formed when the colloidal stability is disturbed and resin droplets are aggregated. The droplet stability is dependent on, for example, pH, electrolyte concentration, viscosity, temperature and also on the chemical composition of the resin (Allen, 1979). The behavior of the different extractive fractions and their individual components in water closure and pulp washing is not well known. In most process studies the extractives have been treated as a single group despite their complex composition and nature.

Extractives can have a serious negative effect on the environment and may also cause problems in the operation of a pulp and paper mill and thus severely affect its productivity. Removal of extractives from the process water (as soon as possible in the beginning of the mechanical process) is important because the extractives are responsible for increased energy consumption in the subsequent refining process. The extractives handling strategy should give an improved paper quality.

Using an Impressafiner it is possible to remove up to 40% of the incoming extractives from the wood chips and it is also possible to reduce the total energy consumption during subsequent refining. The Impressafiner is designed to compress the chips to a uniform size distribution as they proceed to the discharge of the screw press. Inside the Impressafiner there is a high compression ratio which squeezed out extractives both from resin canals as well as from parenchyma cells inside the wood structure.

Extractives which are removed from the process have to be taken care in an economical way. They have to be in a form making it possible to remove them from process water before the water is released from the mill or reused in the mill. In that respect, the extent to which the extractives are present in either a colloidal or fibre-bound phase is important.

The stability of colloidal resin against salt-induced aggregation was studied extensively by Sundberg et al.(1996), Mosbye (2003), Jonhnsen et al. (2004). The results showed that the dissolved substances from unbleached mechanical pulp play an important role in the stability of the colloidal extractives.

The MSc project

The main objective of the work is to study the stability and flocculation of extractives in the process water and the interaction with surfaces. In this way it will be necessary to create model water dispersions (characteristics of the model water dispersion should be close to the water from the Impressafiner) and also to study the behavior of different types of cationic polymers and simple electrolytes on the flocculation behavior of extractives from the model water.

In pure dispersions the colloidal extractives are electrostatically stabilized and can thus be destabilized by addition of simple electrolytes or polymers. However, in the process water extractives are quite stable against electrolyte/induced aggregation because dissolved polymers adsorb to the colloid surfaces and stabilize them. To be able to remove extractives from the process water it should be possible to flocculate them and to use flotation technique (i.e. Dissolved Air Flotation). The loss of colloidal stability will be followed as electrolyte-induced aggregation of DCS and the subsequent sedimentation of the aggregates by gravity or centrifugation using a Turbiscan instrument.

Supervisors: Dr Per Stenius and Professor Øyvind Gregersen

PhD. Student Mihaela Tanase

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