NTNU
Norges teknisk-naturvitenskapelige universitet

Fakultet for naturvitenskap og teknologi
Institutt for kjemisk prosessteknologi

FORDYPNINGSPROSJEKTER HØSTEN 2015
SPECIALIZATION PROJECTS AUTUMN 2015

TKP4510/TKP4511 KATALYSE
(CATALYSIS)

Coordinator: Magnus Rønning

Project proposals from Professor De Chen: *de.chen@ntnu.no*

1. Multifunctional proppants for enhanced oil production from shales

The few last years there has been a significant development in production of oil and gas from shale resources, mainly in the US. Increased supply has resulted in a drop in the gas price in North America and predictions that USA will be self-supplied with oil in the future. The development has been accelerated by progress in two technology areas: horizontal drilling and fracking of the reservoir. During fracking with water at high pressure so-called proppants are added. Proppants are strong particles typically of sand and ceramics that help to keep the fracks (cracks) open. However, regardless of proppant type or the state of fracture, conductivity at the end of the hydraulic fracturing treatment is critical. The fracture conductivity and well performance can be impaired and jeopardized by production related events including inorganic scaling (i.e. deposition of barium sulfate, calcium carbonate, etc.) or hydrocarbon depositions (i.e. paraffin, asphaltenes). Current solutions to these post-hydraulic fracture related production problems include liquid inhibitor additions to the frack fluid, solid inhibitor additives to the proppant slurry, post frack chemical squeezes, downhole chemical injection and periodic clean-outs, among others.
With a composite material between CNT and the traditional proppant, we have a possibility to introduce chemicals (such as a reactant and/or catalyst) directly into the reservoir during fracking for in situ upgrading of the resource. The present work focus on development of multifunctional proppants that provides both designed conductivity and efficient chemical delivery A carbon nanotube or nanofiber layers will be coated on sands. The chemicals such as scale inhibitor will be adsorbed or chemically bonded to the CNT surfaces. The project will comprise synthesis of the composite materials and characterize how these can incorporate a catalyst or reactant. A summer job at the Catalysis group is available.
Supervisors: Prof. De Chen, Prof. Erling Rytter, Dr. Xuezhi Duan,

2. Catalytic conversion of kerogen in enhanced oil production from shales

Oil shale comprises a host rock and kerogen. Kerogen, commonly defined as the insoluble macromolecular organic matter (OM) dispersed in sedimentary rocks, is by far the most abundant form of OM on Earth. Kerogen has a high hydrogen-to-carbon ratio, giving the potential to be superior to heavy oil or coal as a source of liquid fuel. When heated to the right temperatures, some types of kerogen release crude oil or natural gas. Statoil RDI is looking at kerogen as a possible resource for the future Kerogen is an unconventional hydrocarbon source, which is the one of the new focus areas in Statoil. Fundamental understanding of the reaction of depolymerization of kerogen could lead to a more energy effective way for in-situ conversion of kerogen to oils in subterranean geological formations. The present work will test the multifunctional proppants as catalysts for kerogen conversion. The project will also include the characterization of kerogen and the oils produced. A summer job at the Catalysis group is available.
Supervisors: Prof. De Chen, Prof. Erling Rytter, Dr. Xuezhi Duan

3. Kinetic study of oxychlorination process

Catalytic oxychlorination of ethylene with hydrochloric acid and oxygen is the important industrial process to produce 1,2-dichloroethane, which can be converted into vinyl chloride by cracking process. Supported $CuCl_2$ catalyst often used as oxychlorination catalysts. The present work focuses on the catalyst preparation and characterization of K, La and Mg modified $CuCl_2$ layer on alumina supports. The site reactivity will be studied by combined UV-Vis spectroscopy-MS and transient kinetic study on catalysts with different site density. The project will be performed at the catalysis group and be closely cooperated with INEOS.
Supervisor: Prof. De Chen, Kumar Ranjan Rout, Martina Francisca Baidoo and Terje Fuglerud (INEOS)

4. One-pot conversion of biomass to chemicals on Ni-Cu-Zn alloy catalysts

Catalytic processes for conversion of biomass to transportation fuels have gained an increasing attention in sustainable energy production. The biomass can be converted to fuels via three platforms, such as fast pylolysis (bio-oil as intermediate), hydrolysis (sugars as intermediates) and gasification (synthesis gas as intimidates). Recently it has been reported that biomass can be directly converted to polyols, such as ethylene glycol and propanediol. Those polyols can be converted to gasoline and diesels via hydrogenolysis, aldol condensation and hydrogenation reactions on multifunctional catalysts. The project will deal with synthesis, characterization and catalytic test of Ni/Cu/ZnO based catalysts for hydrothermal liquefaction of woody biomass as well as alga. The work will be performed in NorBioLab.
Supervisors: Prof. De Chen, Cornelis Gerardus van der Wijst

5. Catalytic conversion of biomass derived oxygenates to aviation fuels

This project deals with catalytic conversion of biomass derived oxygenates to fuels on multifunctional catalysts integrating the function of aldol condensation, ketonization, oligomerization and hydrogenation. High surface area TiO2 catalysts will be synthesized and characterized for aldol condensation reaction. The Ni-Cu-Zn will be tested as hydrogenation

catalysts. The products will be thoroughly analyzed by GC-MS, HPLC, and work will be performed in NorBioLab.
Supervisors: Prof. De Chen, Cornelis Gerardus van der Wijst

6. Catalysts for lights olefin C_3-C_4 production

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

7. Autothermal dry reforming of methane

Combined total combustion and dry reforming will be studied in a fixed bed reactor. Co/CeO2 will be synthesized, characterized and tested for methane total combustion. Ni-Co catalysts with different Ni/Co ratio will be synthesized and tested for methane reforming. The operating conditions, particular the ratio of $O_2/CO_2/CH_4$ will be studied as a function of activity, CO/H_2 ratio and carbon formation. The catalytic combustion of methane will be focused in the project.
Supervisor: Prof. De Chen, Prof. Anders Holmen, Shirley Elisabeth Liland

8. Catalysts for electrochemical CO_2 reduction

Nanocarbon-Copper based materials are very interesting catalysts for electrochemical reduction of CO_2. Of the pure metals, Copper is the best catalyst for the electrochemical CO_2 reduction. The project will focus on synthesis and characterization of copper nanoparticles supported on graphene. The graphene will be synthesized and functionalized to introduce oxygen and nitrogen groups on the surfaces. Different synthesis methods will be used and compared to achieve the best dispersion of Cu catalysts. The catalysts will be tested by screening of activity and selectivity with a RRDE-setup, while for more precise studies Chronoamperometry with product detection is to be applied.
Supervisor: Supervisor: Prof. De Chen, Ida Hjorth, Yahao Li

9. Synthesis and characterization of tungsten carbide

The project deals with synthesis of core-shell structure tungsten carbide nanomaterials for applications in extra hard materials. Different core materials such as carbon nanotubes, Si carbides will be used for the synthesis. Different synthesis conditions of tungsten carbide will be tested and optimized in terms of phase and wettability with Ni-Cu alloys. The project will be performed at Catalysis Group, Department of Chemical Engineering, NTNU with a close cooperation with Lyn Drilling AS Schlumberger. All the materials will be characterized by different techniques, such as XRD, XRF, SEM, TEM, and mechanical property testing.
Supervisor: Prof. De Chen, Dr. Wei He

10. New catalysts for low-temperature selective catalytic reduction (SCR)

Distribution of liquefied natural gas (LNG) is developing in Norway as well as globally, and represents an option for efficient and more environmentally friendly marine propulsion. Heavy duty engine exhaust from the marine sector constitutes approximately 15% of the total global NOx emissions. State-of-the-art NOx removal from heavy engine exhaust includes selective catalytic reduction where NOx is reduced by a reducing agent such as ammonia (usually generated *in situ* from urea). In transient operation, SCR may be combined with NOx storage in NOx storage and reduction (NSR) systems. Modern engines operate with high fuel efficiencies, and high activity at low temperatures is therefore necessary.
SCR catalysts usually contain an active component (transition metal or PGM) dispersed on a porous support. In addition, a NO_x storage component may be included. γ–Al_2O_3 is often preferred as the support material due to the high thermal stability (<850C°), slight acidity and the capacity to store NO_x at low temperatures. For low-temperature NH_3-SCR, Fe- and Cu-exchanged zeolites are highly promising catalysts. This project aims at investigating modified mesoporous aluminium oxides as catalyst supports for low temperature SCR. Recent studies report periodically ordered mesoporous alumina–tungstophosphoric (HPW) acid composite frameworks that may open up new possibilities for tuning the acidity of the support and to tailor the interaction between the metal function and the support.
The project is affiliated with a new project awarded by the Research Council of Norway TRANSPORT 2025 program. The project work involves synthesis, characterization and screening of catalysts for low-temperature SCR. Development of testing equipment and experimental protocols will be part of the work.
Supervisor/co-advisors: Professor Magnus Rønning, Professor Hilde Venvik, Senior Scientist Rune Lødeng (SINTEF)

11 Reduction of Cu-ZnO water-gas shift catalysts in presence of water

Water-gas shift is one of the most important reactions in the chemical industry, being a key step in processes such as ammonia synthesis. A mixture of Cu and Zn oxides is commercially used to catalyze the low temperature shift reaction (LTS). Typically, the catalyst contains a certain percentage of water due to an incomplete decomposition of the precursors. By reduction of the Cu oxide the active phase (copper metal) is formed. During the reduction water and CO_2 are released. A detrimental effect of the water on the strength of the catalyst is suspected. The aim of this project is to study the effect of steam and pressure (range 10-50 bar) on the crystal size of the copper and zinc oxides, during the reduction of the catalyst. The catalysts will be characterized using techniques such as X-ray diffraction, thermogravimetry, microscopy and Cu surface area measurements using oxidation by N_2O. The work will be carried out in close collaboration with the Yara Technology Centre.
Supervisor: Professor Magnus Rønning. Co-advisors: Sara Boullosa Eiras and David Waller, Yara Technology Centre

12 Efficient catalysts for achieving NO /NO_2 equilibrium

The oxidation of NO to NO_2 is an important reaction in applications such as nitric acid production and selective catalytic reduction (SCR). In nitric acid production, the amount of NO_2 going into the absorption column should be maximised. This can be achieved by using a suitable catalyst. In SCR there is a need for controlling the extent of NO_2 reduction to NO at high temperatures in order to maintain fast SCR reaction conditions.
The project will investigate new catalysts for achieving the NO/NO2 equilibrium for these applications. The work involves synthesis, characterization and screening of suitable catalyst materials, and will be carried out in close collaboration with the Yara Technology Centre. The project is affiliated with iCSI, a Centre for research based innovation (SFI) awarded by the Research Council of Norway to NTNU, with SINTEF and the University of Oslo (UiO) as research partners, and YARA, K.A. Rasmussen, Dynea, INEOS and Haldor Topsøe AS as industrial partners.

Supervisor: Professor Magnus Rønning. Co-advisor: David Waller, Yara Technology Centre

13 Surface modified γ–alumina supports for cobalt Fischer-Tropsch catalysts

The catalysis group at IKP has a long history in research on Fischer-Tropsch synthesis of hydrocarbons from synthesis gas. Much of the work has been in cooperation with SINTEF and Statoil, and has particularly been directed at cobalt catalysts supported on alumina or modified alumina. It has for a long time been known that the catalyst formulation strongly influences the selectivity of the reaction, *i.e.* particularly the amount of C_{5+} components produced. Several factors determining the selectivity has been established, but still there is a mystery why the support in itself has a strong effect, *e.g.* why α–alumina gives more heavy products than γ–alumina.
The strategy of the project is to modify the surface of γ–alumina and thereby investigate the relationship between surface structure and selectivity. Advantage will be taken of the ample amounts of hydroxyl groups on the surface of γ–alumina. By reaction with the-OH groups, the surface properties will be altered, and the effect on the FT-synthesis is to be investigated. The alumina surface will be altered with various molecuels such as trimethylsilyl chloride according to the following surface reaction:

$$\text{S-Al-OH} + \text{ClSiMe}_3 \rightarrow \text{S-Al-O-SiMe}_3 + \text{HCl}$$

thereby giving a silanized hydrophobic surface. Other reactions, like condensation with amines or acids, will also be considered. The reaction path of the anchoring on the surface will be followed by FTIR spectroscopy, TPR and chemisorption before the FT testing

Supervisor/co-advisors: Professors Magnus Rønning, Anders Holmen and Erling Rytter, postdoc Nikolaos Tsakoumis and Rune Myrstad (SINTEF)

14 Fischer-Tropsch synthesis catalysts for CO_2-rich syngas

The project is related to a European project (FASTCARD) seeking to develop new iron-supported Fischer-Tropsch (FT) catalysts in the context of small delocalised 500-3000 bpd biomass to liquids (BTL) plants. The current catalysts need to be improved with respect to high temperature performance, high CO_2 content in the feed, and improved durability.
The aim of this project is to develop catalysts that can operate at elevated temperatures (>250°C) with high carbon efficiency (C_{5+} selectivity). The project will involve synthesis, characterisation and testing of Fe-based FT catalysts. The catalysts will be tested for FT

synthesis activity and also reverse water-gas shift activity (RWGS). The characterisation will involve chemisorption, XRD, TGA-DSC, TPR and S(T)EM.

Supervisor/ co-advisor: Professor Magnus Rønning/ Diego Pena Zapata

15 Doped carbon nanostructures as metal-free catalysts in the oxygen reduction reaction

Platinum group metals (PGM) are targeted by the European Commission as critical materials due to scarce natural abundance in Europe, and insecure international supply. Catalysis is by far the largest industrial use of PGM. Therefore, the development of metal-free catalysts to replace precious metals can represent a real breakthrough in catalysis, particularly for those catalytic processes where a large amount of the active phase is needed. Doped nanocarbons represent a new class of PGM-free catalyst for several potential catalytic applications, including the oxygen reduction reaction (ORR), oxidative dehydrogenation of light alkanes and advanced oxidation processes. The active sites in the metal-free catalysts are strongly embedded into the host matrix. The nitrogen-doped carbon nanofibres (N-CNF) show many properties that are markedly different from those of undoped counterparts. The N-CNF will be synthesized by chemical vapour deposition from a growth catalyst under a mixture of nitrogen-containing hydrocarbons. The emphasis will be put on synthesis methods and characterisation of catalytic activity. The materials will be analysed by a wide range of characterisation techniques such as BET, TGA, XRD, XPS, Raman and STEM.
The work is part of a project funded by EU-FP7 (FREECATS) and is a collaboration with academic and industrial partners from several European countries.
Supervisor/co-advisors: Professor Magnus Rønning/ Marthe Emelie Buan

Project proposals from Professor Hilde J. Venvik: *hilde.venvik@ntnu.no*

16 Characterization of Ag catalysts for formalin production

Formaldehyde is the essential component of wood adhesives for a wide range of applications and an important intermediate in the production of many fine chemicals. Formaldehyde is produced via selective catalytic oxidation of methanol to formaldehyde. Dynea is a Norwegian based producer of specialized adhesives and coatings, and global licensor of formaldehyde technology. Oxidation over a silver (Ag) based catalyst in excess methanol is identified by Dynea as the preferred technology in terms of minimizing investment, energy consumption and operating cost with further potential for improving profitability by increasing the product yield. The project aims at establishing a suitable characterization methodology for Ag based catalysts. Results from fresh and plant exposed catalysts supplied by Dynea will be analysed and compared, with an overall objective to identify factors critical to the selectivity and stability. A wide range of characterization tools will be evaluated, such as scanning electron microscopy (SEM) and transmission electron microscopy (TEM), x-ray photoelectron spectroscopy (XPS), depth profiling by Auger electron spectroscopy (AES) under Ar ion sputtering, x-ray diffraction (XRD), scanning probe microscopy (SPM), infrared (IR) and Raman spectroscopies, thermogravimetric analysis (TGA), temperature programmed reduction/oxidation/desorption/etc. (TPX).

The project is affiliated with iCSI, a Centre for research based innovation (SFI) awarded by the Research Council of Norway to NTNU, with SINTEF and the University of Oslo (UiO)

as research partners, and YARA, K.A. Rasmussen, Dynea, INEOS and Haldor Topsøe AS as industrial partners.

Supervisor: Prof. Hilde Venvik
Co-advisors: Senior Scientist John Walmsley (SINTEF), Senior Scientist Rune Lødeng (SINTEF). Dynea personnel will also be engaged in the project.

17 Catalysis for control of methane slip in marine machinery

Distribution of liquefied natural gas (LNG) is developing in Norway as well as globally, and represents an option for efficient and more environmentally friendly marine propulsion. With LNG as fuel, it is critical that methane emissions (methane slip) are cut to very low levels since methane is a greenhouse gas with 20 times the global warming potential of CO_2. Moreover, a comparable or higher overall efficiency is required to enable reduced CO_2 emissions relative to other marine fuels. Measures that seek to reduce NOx formation or CH_4/NOx clean-up should hence not compromise the efficiency. Catalysts for methane slip abatement therefore need to facilitate complete oxidation of CH_4 to CO_2 and H_2O at highly diluted methane concentrations and moderate temperatures. The most active catalysts are usually based on supported noble metals (Pd, Pt), but measures to replace (part of) the costly components are being explored.

The project is affiliated with a new project awarded by the Research Council of Norway TRANSPORT 2025 program. The activities involve synthesis, characterization and testing of catalysts for methane oxidation under application relevant conditions. Modification of existing equipment and establishment of suitable experimental protocols will be part of the work.
Supervisor: Prof. Hilde Venvik
Co-advisors: Senior Scientist Rune Lødeng (SINTEF), Prof. Magnus Rønning.

18 Direct conversion of methane to C2 hydrocarbons, aromatics and hydrogen.

Methane activation by heterogeneous catalysis will play a key role to secure the supply of energy, chemicals and fuels in the future. Methane can be converted to chemicals and fuels in two ways, either via synthesis gas or directly into C_2 hydrocarbons and methanol. Today, almost all commercial processes for large scale natural gas conversion involve synthesis gas. However, the direct conversion without going through syngas represents a “dream reaction”. The present approach focuses on the non-oxidative one step conversion of methane into C_2, aromatics and hydrogen. It has recently been shown (Science 344 (2014) 616) that methane can be converted at high temperature on catalysts containing single iron sites in a silica matrix. The project explores catalyst preparation, characterization and testing in a suitable reactor based on the above results from Science.

Supervisors: Anders Holmen and Hilde J. Venvik, Dept. of Chemical Engineering (IKP), Bjørn Chr. Enger (SINTEF) (Hilde.Venvik@chemeng.ntnu.no)

19 Initial stages of metal dusting corrosion

Metal dusting is a high temperature corrosion phenomenon that constitutes a problem in the conversion of natural gas to fuels and chemicals because it causes a gradual breakdown of

alloy surfaces into fine, dust-like particles. It is a result of unwanted carbon formation on the inner surface of process equipment, and occurs where metals and alloys are exposed to a gaseous atmosphere with low oxygen/steam partial pressure at elevated temperature (300 ºC and up). This is typical for the production of synthesis gas from methane. Metal dusting carries significant cost, since precautions need to be taken to avoid catastrophic events in industrial processes characterized by explosive and/or poisonous gaseous mixtures under high pressure and temperature.

The progress of metal dusting in the alloy matrix once carbide phases have formed has been well studied and documented. The initial stage of metal dusting is, however, analogous to the carbon formation on catalysts used in the production of synthesis gas, but less described. Carbon formation on catalysts is essentially kinetically controlled, particularly facile on Ni, Co and Fe, and has been widely studied. Fe and Ni are common constituents of alloys with good temperature resistance; hence their stability in the alloy matrix is critical for metal dusting. The overall objective of this study is to obtain better understanding of the initial stages in metal dusting corrosion, i.e. the initiation of the carbon formation. This is done by preparing different surface oxides of a representative alloy, which is then exposed to high carbon activity gas atmosphere at high temperature. This is combined with advanced characterization before and after the exposure in order to find a relationship between the structure and composition of the alloy surface and its propensity to form solid carbon. The project work will focus on alloys applied in so-called microstructured reactors (Inconel 800 series) for process intensification, and the particular issues associated with such reactors.

Supervisor: Prof. Hilde Venvik
Co-advisors: Research Scientist John Walmsley (SINTEF), Post doc. student Daham Gunawardana. PhD student Xiaoyang Guo. Possible collaboration with Karlsruhe Institute of Technology.

20 Direct and indirect synthesis of DME over acidic catalysts.

Dimethyl ether (DME), CH_3OCH_3, is the simplest ether and a possible clean and economical fuel for the future, with the characteristics of a sulphur free diesel fuel with low particulate emissions and high cetane number. The properties of DME are similar to those of LPG and it can hence be used for power generation as well as residential heating and cooking. DME is currently produced in a two-step process; a methanol synthesis step followed by the methanol dehydration reaction. DME production from syngas is thermodynamically more favourable than from methanol and the direct DME synthesis should thus be more economic, provided a suitable catalyst is identified and combined with the appropriate reactor technology. At NTNU, we have successfully applied so-called microstructured reactors with integrated heat exchange for the direct synthesis of DME over physical mixtures of a Cu-based methanol synthesis catalysts and an acidic (γ-alumina, HZSM5) methanol dehydration catalyst. The project aims at modifying the activity and stability of different dehydration catalysts, and possibly to compare them in the direct synthesis and the dehydration alone. The work includes synthesis, chemical treatment, characterization and testing of catalysts in a high pressure experimental set-up. The project is part of a collaboration with SINTEF Materials and Chemistry.

Supervisor: Prof. Hilde Venvik
Co-advisors: Prof. Anders Holmen, Research Scientist Rune Myrstad (SINTEF), PhD student Farbod Dadgar, postdoctoral fellow/senior engineer Cristian Ledesma

21 Microchannel membrane reactor for small scale hydrogen production

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

We recently showed that the membrane's permeability under pure hydrogen as well as its sensitivity to carbon monoxide (CO) could be changed (reduced) through a particular heat treatment, and this has important implications for their applicability. The microchannel configuration is particularly suited for investigations of these phenomena. The topic involves investigation of the effect of relevant co-molecules such as CO, CO_2, H_2O, CH_4, and CH_3OH in the membrane microchannel configuration through experiments and modelling, as well at characterization of surface species present on the membrane during and after permeation experiments. The work will be carried out in collaboration with SINTEF Materials and Chemistry in Oslo.

Supervisor: Hilde Venvik
Co-advisor: Dr. Thijs Peters and Dr. Ingeborg-Helene Svenum (SINTEF).

22 Process intensification of the Fischer-Tropsch synthesis

In the Fischer-Tropsch (FT) synthesis, synthesis gas (H_2+CO) can converted to liquid hydrocarbons, and the technology is currently applied in large-scale plants to produce fuels and oils from natural gas. Microstructured reactors are under development for process intensification, i.e. enhancement of productivity per mass or volume of the reactor, and such devices are considered particularly interesting for off-shore conversion (FPSO) of associated gas or conversion of biomass to fuels. At NTNU, we recently published very interesting results on FT synthesis over a Co-based catalyst in a microstructured reactor with integrated heat exchange. This project is a continued study, with emphasis on further investigations of this reaction environment in terms of pressure, temperature and synthesis gas composition. In particular, unresolved selectivity effects related to high pressure (>20 bar) may be addressed, as well as issues related to the lower deactivation rate observed in the microchannel reactor compared to fixed bed experiments under otherwise equal conditions. Another possible direction is the development of catalysts – Fe or Co based – that fit the properties of the reactor. The project is part of a collaboration with SINTEF Materials and Chemistry.

Supervisor: Prof. Hilde Venvik
Co-advisors: Prof. Anders Holmen, Research Scientist Rune Myrstad (SINTEF), Research Scientist Jia Yang (SINTEF).

TKP4520/4521 KOLLOID OG POLYMERKJEMI (COLLOID AND POLYMERCHEMISTRY)

Coordinator: Johan Sjöblom

Project proposal from Professor Johan Sjöblom: *johan.sjoblom@ntnu.no*

23 Amino-functionalization of magnetic nanoparticles for extraction of naphthenic acids from model oils

Main project activity for the fall semester includes writing a literature review on various types of the magnetic nanoparticles, functionalization mechanisms and their possible use for the naphthenic acid removal from model and crude oils.
Main supervisor: Prof Johan Sjöblom Co-supervisor: Dr Galina Rodionova

24 Emulsions in porous media

The behaviour of emulsions in porous media is a central topic in all aspects of EOR. With right properties of the emulsions there will be no flow restrictions regardless of the difference in sife of porous. In this project we prepare different swelling / non swelling porous materials and design a variety of emulsion properties with regard to elasticity / viscosity of the interfacial region. The characterisation part of emulsions and porous material will be essential. Experimental techniques will involve NMR, BET, interfacial rheology.
The supervisor team will consist of : Johan Sjöblom, Camilla Dagsgård and Geir Sørland

25 Destabilization of asphaltene and particle-stabilized emulsions

Classical destabilization of w/o emulsions is to use chemical demulsifiers. In this way the crude oil is purified and export qualities can be achieved. However, in many cases like heavy crude oil, the chemical demulsification is not enough and a combination of chemicals and electric fields is applied.
In this project w/o emulsions with high stability are prepared and sets of chemicals and electric fields are applied for destabilization. The stability is monitored by a set of techniques like low field nuclear magnetic resonance (LF-NMR) and the Ecritical technique. The project is supervised by Prof. Johan Sjöblom and Dr. Sébastien Simon at Ugelstad Laboratory and is a collaboration with Wärtsilä Oil and Gas.

26 "Interactions between Asphaltene Fractions"

Asphaltenes are a heavy polar fraction of crude oil, giving rise to organic deposition phenomena in reservoirs, wells, piping and equipment. Unabated asphaltene deposition leads to costly production flow restrictions as well as costly unplanned production outages. Consequently it is important to determine the properties of asphaltenes to be able to optimize treatment to prevent deposition.
A procedure to separate asphaltenes into several fractions of different properties has recently been developed. The goal of this Master project is to study and quantify the interactions between these fractions. These interactions will be studied by techniques like Isothermal Titration Calorimetry (ITC), Near-Infrared measurements and fluorescence.

This project is a part of the *Joint Industrial Program "Improved Mechanisms of Asphaltene Deposition and Precipitation to Minimize Irregularities in Production and Transport – A Cost Effective and Environmentally Friendly Approach"*, a project sponsored by the Norwegian Research Council and several central oil companies and chemical vendors. The work will be done at Ugelstad Laboratory, Department of Chemical Engineering and the supervisors will be Dr. Sébastien Simon and Pr. Johan Sjöblom.

27 Influence of molecular complexation on partitioning of acidic components between water and oil

The project will investigate to what extent a molecular complexation (acid-base, H-bonding…) in the oil phase will influence a distribution (partitioning) of fatty acids between oil and water. Technically this is an important issue for pH determination and process modelling. The partitioning will be experimentally measured by High Performance Liquid Chromatography (HPLC).
The project is supervised by Prof. Johan Sjöblom and Dr. Sébastien Simon at Ugelstad Laboratory and is a collaboration between Ugelstad Laboratory and industry.

Project proposals from Professor Gisle Øye: *gisle.oye@ntnu.no*

28 Influence of Enhanced Oil Recovery (EOR) chemicals on produced water treatment. Interfacial characterisation of gas-liquid interfaces related to gas flotation

Breakthrough and subsequent back production of EOR chemicals (surfactants and/or polymers) will have strong impact on the amount of dispersed oil in produced water. Many produced water treatment systems are designed to handle produced water from conventional water flooding, but cannot satisfactorily handle produced water from chemical flooding. This is particularly challenging offshore were current methods are not efficient nor compact enough to reach discharge or reinjection quality of the produced water.

Gas flotation, i.e. attachment of oil and particles to gas bubbles, is a common treatment method for removing dispersed oil produced water streams. The interfacial properties of gas bubbles will influence the efficiency of this method, and it is clear that the presence of EOR chemicals (surfactants and polymers) will influence gas-water interfaces.

The aim of this project will be to study how EOR chemicals influence the interfacial tension between produced water and gas bubbles at short time scales. The interfacial tension measurements will be carried out utilizing a maximum bubble pressure tensiometer.

Supervisors: Sirsha Putatunda and Gisle Øye

29 Preparation of nanostructured TiO_2 surfaces

TiO_2 nanostructures include nanotubes, nanorods, nanowires, nanodots as well as nanoporous films. All these structures can be composed of pure phase or bi-phase TiO_2, usually after transformation from the amorphous phase depending on annealing temperature. These nanostructures may improve electron transport through photocatalytic films as well as provide large surface areas for the adsorption of pollutant. Conventional TiO_2 photocatalysis has barriers in practical remediation of organic pollutants due to the low efficiency in sunlight absorption. In general, visible light photocatalysis on TiO_2 can be facilitated by introducing additional electronic states and higher activity can be realized by creating electronic interactions between TiO_2 and modifying materials (dye, noble metal, narrow band semiconductor, etc.). Anodic oxidation of titanium layers seems to be the more convenient approach in order to create self-organized 3D titania nanostructured layers with strong adhesion, mechanical stability and no defects (i.e. ensure that the recombination rate of the photo-generated electron-hole pairs is lower). This technique is a simple, highly reproducible and low-cost approach compared to expensive and time-consuming lithographic or epitaxial methods.

The aim of this project will be to prepare TiO_2 nanostructured surfaces by anodic oxidation. Scanning electron microscopy (SEM) will be used to characterize the synthesized structures. The experimental work will be carried out at Brno University of Technology (BUT) in Czech Republic.

The project is part of the Czech-Norwegian Bilateral Scholarship Programme.

Supervisors: Jana Drbohlavová (BUT) and Gisle Øye (NTNU)

Project proposals from Associate Professor Brian Grimes: *brian.grimes@ntnu.no*

30 Multi-scale modeling of interfacial mass transport in emulsions

This project employs molecular dynamics (MD) simulation and a continuum mass transport model to predict interfacial concentrations of surfactant molecules in liquid-liquid dispersions (emulsions). The student will learn the basics of MD and construct molecular simulations of surfactant adsorption at a liquid-liquid interface. The MD calculations are used to parameterize an adsorption isotherm employed in a continuum interfacial mass transport simulation. The student will use this MD parameterized continuum model to simulate multi-component adsorption in an emulsion to calculate the interfacial concentrations of the surfactants based on the initial surfactant composition of the oil and the emulsion parameters. The application is orientated towards model crude oil-water emulsions with synthetic crude-oil surfactants or purified indigenous crude oil surfactants.

31 Molecular simulation of adsorbed surfactant interactions during coalescence

The presence of adsorbed surfactants such as asphaltenes at liquid-liquid interfaces can lead to steric interactions that induce a positive disjoining pressure which significantly slows down the coalescence process. In this project, MD simulations of synthetic asphaltenes at liquid-liquid interfaces will be performed at various levels of surface coverage and interfacial separation distances to determine the pressure and interaction energies in the liquid film between the interfaces. The student will learn the basics of MD simulation and coalescence theory as well as learn how to set up MD simulations for interfacial systems and analyze the results.

32 Population balance modeling of interfacial mass transport during coalescence and breakage

The dynamic evolution of the drop size distribution of an emulsion in transport and separation processes that occurs due to drop-drop coalescence and drop breakage can significantly change the surface-to-volume ratio of the emulsion. This evolution of the surface-to-volume ratio will consequently lead to changes in the interfacial composition of adsorbed surfactants which can alter the dynamics of the coalescence and breakage processes. Therefore, in this project a model will be developed that couples an interfacial mass transport model to a population balance model for coalescence and breakage and a code will be developed to solve the model. The student will learn basic approaches for numerical solutions of partial differential equations and should be confident with basic transport phenomena theory and computer programming.

Project proposals from Associate Professor Kristofer Paso:

kristofer.paso@ntnu.no

33 Rheological Properties of Waxy Crude Oils and Waxy Emulsions

Gelling of waxy produced hydrocarbon fluids is a major problem for producers when flow in oil pipelines must be shut-in due to scheduled maintenance or emergency situations. NTNU has developed a pipeline restart simulator which tracks the pressure wave propagation process when the gelled pipelines must be restarted. Initially, an acoustic sound wave travels along the pipeline, distributing pressure according to the yield stress of the waxy gel. Then, a coupled viscous compression wave and gel degradation wave travels along the length of the pipeline, and extending the distance which the pressure wave can travel and allow restart. Restart occurs after the pressure wave is reflected off the outlet end of the pipeline, and large scale flows commence throughout the pipeline.

The master's students project will be to extend the understanding of waxy oil and waxy emulsion rheology to gas condensate fluids and complex fluids. The following understanding of the process will be studied by the student: (1) Solid Fraction Dependence of Rheology Parameters, (2) Aging Processes for long-term shut-in, (3) Gelation Kinetics, (4) Gelation during shear to emulate forced shut-in flows, and (5) Herschel-Bulkley exponent impact. The methods will primarily be rheometry, DSC, TGA, and microscopy. The instrumentation is available and in working condition at Ugelstad Laboratory. In addition, the master's student will become familiar with the relevant industries which support the pipeline restart research.

Qualifications: Current master's student in chemical engineering or related discipline.

Advisor: Associate Professor Kristofer Paso, email: kristofer.paso@ntnu.no

34 Liquid Crystals for CO2 Capture and Storage

A new concept is developing for an integrated CO2 capture, transport and storage process using nano-structured solutions suitable to capture CO2 via absorption at localized CO2 sources. After the nanostructured solutions are saturated with CO2, they are injected into aquifers and ensure dual sealant mechanisms against CO2 leakage. The nanostructured solutions constitute a durable thermodynamic sealant mechanism against CO2 leakage. Caprock constitutes a second sealant mechanism against CO2 leakage out of the aquifers. Nanostructured solutions contain cylindrical nano-geometries in aqueous media, providing optimal phase ratios for CO2 capture processes. The new concept offers a novel method to capture CO2 in a transportable medium. Transport risks are minimized because the nanostructured solutions are water-based and can be easily pumped and further diluted to prevent plugging. Storage risks are minimized with dual sealants. In comparison to conventional CO2 capture processes, the new concept requires less compressive energy in order to capture the CO2 in an overall liquid and flowable form. Thereby, the new concept has the potential to provide significant overall energy and cost savings.
Activities in the fall project for the master's degree student will involve anionic or other living polymerization reactions for synthesis of block copolymers, as well as possible modification of commercial block copolymers. Single or multiple step synthesis protocols may be used to create covalently linked hydrophilic and hydrophobic blocks with designated functionalities to provide CO2 uptake with favorable performance. Methods of X-ray diffraction, NMR, light scattering, and rheometry will be used to characterize self-assembled block copolymer structures in aqueous solution.

Qualifications: Current master's student in chemical engineering or related discipline.

Advisor: Associate Professor Kristofer Paso, email: kristofer.paso@ntnu.no

35 Nanoparticle-based wax inhibitor development

A new generation of paraffin wax inhibitors will be developed for the oil and gas industry, based on modified silica nanoparticles. The primary activity mechanism of the inhibitors will be morphological modulation, effecting compact spheroids with reduced propensity to gel. A secondary mechanism will be steric/entropic repulsion, providing dispersion stability against irreversible aggregation. The research program will comprise functionalization of silica-based nanoparticles, co-formulation with known effective comb-polymers, and performance assessment via rheological measurements and differential scanning calorimetry (DSC). In parallel to the verification of inhibition performance, environmental properties of the nanoparticles will be assessed using a comprehensive production-tracking approach. Aqueous dispersion (resulting from polar component adsorption) and hydrocarbon re-extraction experiments will be performed to emulate production flows from the wellhead and through separation equipment. Preferential quantitative partitioning will be demonstrated to the hydrocarbon phase, minimizing adverse environmental impact. The impact of nanoparticles on hydrocarbon dispersion into seawater will be assessed and quantified. In addition, impact of the nanoparticle system on hydrocarbon recovery

efforts will also be assessed and quantified, including water uptake processes and consolidation. Finally, a particle recycling system will be developed to improve environmental sustainability, reduce environmental contamination and promote treatment of refining waste streams. Thereby, a comprehensive approach will be used in assessing environmental properties of new nanoparticle inhibitors.
The methods will primarily be Malvern Zetasizer Nano ZS, Turbiscan, rheometry, DSC, TGA, and microscopy. The instrumentation is already available and in working condition and maintained by technicians at Ugelstad Laboratory.

Qualifications: Current master's student in chemical engineering or related discipline.

Advisor: Associate Professor Kristofer Paso, email: kristofer.paso@ntnu.no

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TKP4530/TKP4531 MILJØ- OG REAKTORTEKNOLOGI (ENVIRONMENTAL ENGINEERING AND REACTOR TECHNOLOGY)

Coordinator: Hanna Knuutila

Project proposals from Associate Professor Hanna Knuutila,
hanna.knuutila@ntnu.no

36 Strong bicarbonate forming solvents for absorption of CO_2

This work is part of EU-project Hipercap (**http://cordis.europa.eu/projects/rcn/111440_en.html**).

Bicarbonate forming systems are interesting partly because they may have a high capacity to bind CO_2 and, because it may be relatively easy to regenerate the CO_2 from the solvent. Based on this observation, it can be envisaged that bicarbonate formers with stronger basicity can lead to increased performance. In this project two promising solvents identified in the Hipercap project are investigated. The activities listed below is for students. The activities are

- Measure the volatility two bicarbonate forming solvents. The volatility is important characteristic of the solvent and is needed to estimate the volatility losses of the solvent. The volatility will be measured in Ebuilliometer up to 100^{o}C.
- Model the equilibrium of measured amine-water system (binary VLE).
- Determine experimentally the protonation constant, pKa. The pKa values are measured by titration up to 80-90^{o}C. This equilibrium reaction property is important in the design of new solvent systems and is needed for accurate kinetic and thermodynamic modelling of absorbers and desorbers.
- Measurement vapor-liquid equilibrium of amine-CO_2-water system. We have already some data but more experimental data is needed to better understand the system behavior.

The autumn project is planned continued to an MSc thesis, but not necessarily in the same area. During the master theses one option could be to use the measured data together with literature data to fit a rigorous thermodynamic model for tertiary systems (amine-CO_2-water).
Supervisors: Ardi Hartono and Hanna Knuutila

37 Combined H_2S removal and hydrate control

This work is part of phd-student project funded by Gas technology centre NTNU-SINTEF. The removal of small amounts of H_2S is often a problem associated with natural gas treatment. In this study new regenerative solvents for H_2S removal are experimentally studied. The experimental work is based on screening experiments where gas with known composition is bobbled through a selected solvent solutions and the amount of H_2S absorbed is measured. The objective is to study the influence of solvent concentration, absorption temperature and H_2S concentration on the absorption behavior. If time allows the influence of CO_2 in the gas phase is additionally investigated.
Supervisors: Hanna Knuutila and Usman Shoukat (PhD-student)

38 Simulation of H_2S removal at high pressures using ASPEN PLUS

The removal of small amounts of H_2S is often a problem associated with natural gas treatment. In this project the ultimate objective is to investigate the feasibility of H_2S removal from natural gas in subsea using a generative system. To be able to estimate the how trustful the simulation results are the work will start with H_2S removal. The activities during the autumn project are:

- Collection of experimental data available in the literature
- Validation of the vapor liquid model describing H_2S-amine system in ASPEN PLUS
- Study the influence of H_2S concentration and amine concentration on H_2S capture
- Study the influence of presence of CO_2 in the gas phase.
- Investigate the stripper configurations and process conditions. (if time allows)

The autumn project is planned continued to an MSc thesis with focus of process development for subsea operation.

Supervisor: Hanna Knuutila

39 Measurement of vapor liquid equilibrium in SO_2 absorption

Professor Olav Erga has been working on a process for SO_2 removal from industrial exhaust gases more than 30 years. The process is based on chemical absorption. Two industrial scale plants are built based on this technology. One plant is built in New Jersey, while the other is built for the Italian energy company ENI at the Sannazarro refinery in Italy. For process optimization more vapor liquid equilibrium data for the SO_2-solvent -system is needed. Additionally there is need for physical property data like densities and viscosities. The activities in this autumn project are:

- Validation of the VLE method used for measurement of VLE
- Measurement of vapor-liquid equilibrium up to temperatures 120^{o}C.
- Measurement of density and viscosity of the solutions.

Supervisor: Hanna Knuutila

40 CO_2 absorption: Calorimetric measurements

One of the most important properties of new absorbent systems for CO_2 capture, are their thermal behavior. To estimate the energy requirement of process based on chemical absorption, the heat of absorption of the solvent as function of temperature and CO_2 content is needed. In the resent year many novel solvents have been proposed which undergo phase chance during absorption of CO_2. With precipitating systems the data interpretation is more challenging, since both absorption and solidification happens at the same time. In this work the heat of absorption of solvent systems undergoing phase change is measured from 40 to 120^{o}C. The study will focus on the reproducibility of the data and comparison of different solvents. Additionally the possibility to use the total experimental pressure data, recorded during the experiments, to estimate the vapor-liquid equilibrium of the system will be evaluated.

Supervisors: ***Inna Kim (SINTEF) and Hanna Knuutila***

41 Kinetics and physical solubility in CO_2-absorbent systems

We have three kinetic apparatuses, one wetted wall column(WWC),a string of discs(SDC) and a stirred cell. Mass transfer rates will be measured for both CO_2 loaded and unloaded system to provide an experimental basis for developing kinetic models. These models can be based on simplified concentration based equilibrium models or activity based using the more rigorous e-UNIQUAC or e-NRTL. Physical solubility of CO_2 into the solvent in addition to density and viscosity are necessary data for the kinetic modelling and will be measured. Physical solubility measurements are based on the so called N_2O analogy.

Supervisors: ***Hanna Knuutila and Ugo Aronu (SINTEF)***

42 Gas (N_2O/CO_2) Solubility into water at moderate pressure

Gas solubility in any solvent is very important in gas processes/ gas separation industry. The process is governed by equilibrium condition either physical or chemical equilibriums between gas and liquid. The measured equilibrium data then becomes crucial and very important in designing gas contactor. Autoclave is one of Vapor liquid equilibrium apparatuses, commonly used. The results are often calculated from mass balance and measured pressure and temperature data. However, measuring concentrations both in gas and liquid phases would give needed information for modeling and predicting the solubility of gas in the liquid. Planned activities are

- Measurement of gas (CO_2/ N_2O) solubility in water at different temperatures and pressures.
- Measurement of gas (CO_2/ N_2O) concentrations in gas/ liquid phase by using GC analyzer during the experiments.
- Comparison of measured data with literature data.
- Thermodynamic modeling of the measured P,T,x,y data using an Equation of State (EOS)

Supervisors: Ardi Hartono, Inna Kim and Hanna Knuutila

43 Measurements and modeling of physical properties of solvents at high pressure

Design and operation of the gas liquid contactor requires physical properties of the studied solvents. Viscosity of solvent is one of important physical property where it relates directly to a mass transfer property as well as a transport property. We have used a rheometer (Physica Anton Par MCR 100) to measure viscosity at ambient pressure. We have expanded the ability of this apparatus to measure at higher temperature (up to150C) and higher pressure (150bar).
Planned activities:
Development and verification of the experimental procedure for viscosity at high pressure measurements
Measurements of solvents properties at different concentrations, CO2 loadings, temperatures and pressures
Modeling (fitting) of the measured properties

Supervisors: Ardi Hartono and Hanna Knuutila

44 Degradation modelling

During plant operation the solvent amine will slowly degrade to other chemical compounds due to the presence of CO_2 and O_2 in the gas phase in the absorber. There are more than 20 degradation components identified for the benchmark solvent 30wt% MEA. To better understand the degradation a model has been developed (Matlab) in our group. The model is fitted to data from lab scale experiments. The objective of this work is to improve and expand the model. The activities are:

- Critical evaluation of the new experimental data and comparison with old data
- Expand the model to better describe the experimental data
- Fitting the model with the more data
- Evaluation of the results.

Supervisor*: Hanna Knuutila*

Project proposals from Professor Jens-Petter Andreassen:

jens-petter.andreassen@ntnu.no

45 Project assignments in hydrometallurgy

Production of metals and other materials based on minerals are believed to be the future industry in Norway after oil and gas. Together with the industry companies, Yara, Glencore Nikkelverk and Boliden Odda we are starting up projects for how to remove different impurity compound from process solutions based on mineral raw materials and before the production of metals or removing trace compounds from calcium phosphate raw material for fertilizer production. Both literature studies and lab work will be offered.

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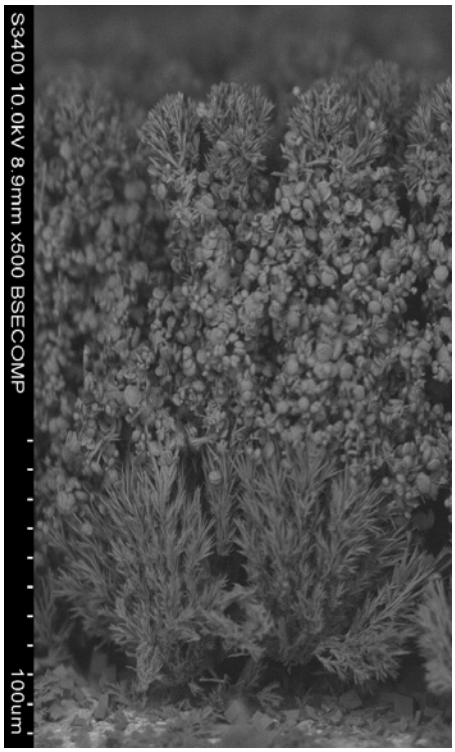
46 Scaling of calcium carbonate on heated surfaces.

During production of natural gas, calcium ions originating from the reservoir fluids and carbon dioxide from the gas phase can react to form calcium carbonate, either as particles in the bulk liquid or as surface scaling on the process equipment onshore. The calcium carbonate scale acts as an insulator on heat exchangers, and frequent shut-downs are required to remove this scale. Scaling is therefore a major challenge in many parts of the industry and the control or prevention of this phenomenon represents a huge economic and environmental advantage. Scaling and bulk precipitation will be studied in a set-up with continuous addition of reactants at constant composition conditions by varying the concentration of calcium, the temperature difference of the liquid bulk and the scaling surface and the surface treatment of the scaling surface. The composition and growth rate of the scale will vary with the experimental conditions and characterization will be performed by SEM and XRD.

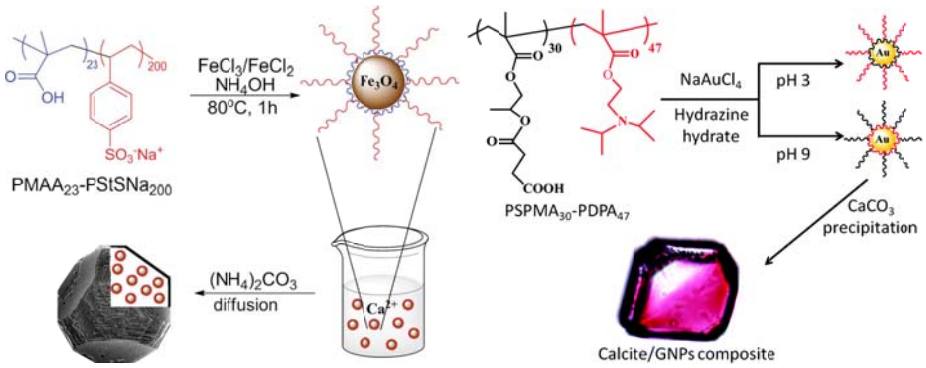
Reserved for Therese Bache, but similar projects can be made.



Different calcium carbonate scale layer structures on top of a heated steel surface.

47 Incorporation of nanoparticles and molecules inside crystals

Recent findings in the literature have shown that nanoparticles can be incorporated inside larger crystals, thereby changing the properties of the crystals and giving new hybrid materials. This is a hot topic both because of the potential use of the new materials but also because crystallization is traditionally seen as a method of purification that would not allow incorporation of molecules or nanoparticles in the crystal. The project will investigate change in the colour and for instance magnetic properties of the crystals by incorporation of different particle/molecular systems. We will investigate the. Relevant crystals will be calcium carbonate and calcium phosphate that are found as biominerals in Nature, where different hybrid materials are also found. The thermodynamic driving force for their formation and hence the growth rate will be changed to see if this is the determining factor for incorporation, one of the key questions in this research. A number of solid characterization techniques will be used and some of the work can be performed in the Nanolab, especially if the work is continued to MSc.



The figure shows magnetic and colored crystals of calcium carbonate (images from the Meldrum group, University of Leeds) due to incorporation of magnetic nanoparticles (magnetite) or gold nanoparticles (GNPs).

Project proposals from Professor May-Britt Hägg, *may-britt.hagg@ntnu.no*

48 Pilot scale testing of fixed-site-carrier hollow fibers for CO_2 capture from flue gas - innovation projects with industry (1) oil producers, and 2) cement industry

There are two projects within this field as indicated above, and thus available for 2 students

The intergovernmental panel on climate changes (IPCC) report from 2007, states that human activities contribute to climate change, furthermore that the largest contribution originates from emissions of carbon dioxide (CO_2) by burning of fossil fuels. Globally, industry is responsible for one-third of all energy consumed, and all together almost 40% of total world CO_2 emissions. Concern for consequences of a rising temperature and climate change inquire new technologies to meet the growing energy demand and increasing world population. A solution for reducing the greenhouse gas emissions to the atmosphere is carbon capture and storage (CCS). Storing highly pure and compressed CO_2 underground in geological formations may be a possible solution. Chemical absorption processes are fully matured to achieve sufficient capture of CO_2, but still struggle with issues like high energy consumption and amine deactivation. The membrane technology offer an energy-saving, low cost, easy operation and smaller footprint than absorption, and are therefore being recognized as an alternative for CO_2 capture.
However, to compete with absorption, membranes must overcome the traditional membrane separation trade-off between permeability and selectivity for CO_2. Facilitated transport membranes have experienced a breakthrough that can overcome this obstacle. By developing composite membranes, which have an ultra-thin selective layer with facilitated transport properties, the separation performance increases drastically.

The main objectives for these two projects are:

- to participate in preparing pilot scale composite hollow fibers modules (both projects),
- to participate in and test on performance when installed at the Tiller plant *(the oil industry project).*
- to participate in the engineering part of an experimental rig (*the cement plant project*), cost estimations, commissioning of rig with membrane modules; process simulations

The hollow fiber modules to be used are based on polysulfone (PSF) as porous support and selective layer of polyvinylamine (PVAm) for CO_2 from flue gas. The modules to be coated are received from Air Products (USA) through these collaborative project.

For both projects a review of the literature for fixed-site carrier membranes, coating techniques and gas separation properties of composite hollow fibers, should be performed.

The experimental work will consist of (work will be adjusted according to available time):
Coating and testing the pilot scale hollow fiber modules based on given preparation parameters (polymer concentration, pH solution, drying time, temperature and packing density).

Co-supervisors: Dr. Xuezhong He and Dr. Arne Lindbråthen (NTNU)

49 Process simulation of Fixed-site-Carrier Polyvinylamine (FSC-PVAm) Membrane for CO_2 capture.

Phase 2: Scaling-up the membrane module to pilot size

Global warming is becoming a world challenging issue related to the emission of greenhouse gases (GHG), especially CO_2. Three different options could be used for the reduction of CO_2 emissions, i.e., improve the energy efficiency of the processes, reduce fossil fuel consumption and CO_2 capture and storage (CCS). The key attraction of CCS is that we may continue to use fossil fuels without causing significant CO_2 emissions, which would be a most promising way to reduce the CO_2 emissions as required by the Kyoto protocol. Chemical absorption processes are fully matured to achieve sufficient capture of CO_2, but still struggle with issues like high energy consumption and amine deactivation. The membrane technology offer an energy-saving, low cost, easy operation and smaller footprint than absorption, and are therefore being recognized as an alternative for CO_2 capture. The facilitated transport, on which the FSC-PVAm membrane is based, is quite challenge as it is a combination of both the standard solution-diffusion and enhanced transport based on a chemical reaction. The process conditions will heavily influence which mechanism is dominating. There is no simulation tool available today which in a good way take both into account. The existing in-house simulation program at NTNU, Chembrain (interfaced to HYSYS) is based on the solution-diffusion mechanism, even though it has been used to give fairly good results in the low pressure range.

The goal of the project is to incorporate the chemical reaction in the current Chembrain code from the mass transport, getting a suitable simulation tool for the facilitated transport through the membrane. (The code should be written in Visual Basic language). Some experimental tests for validation may be relevant.

The candidate must be interested in/ having the background for programming and simulations

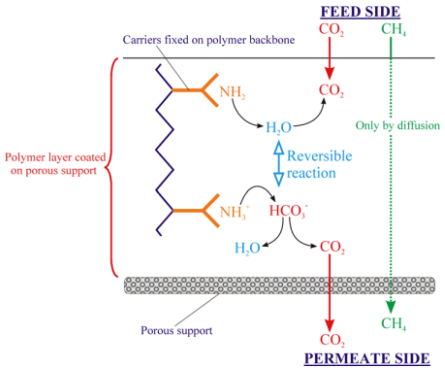


Fig 1. A proposed mechanism of facilitated transport in a fixed-site–carrier membrane

Co-supervisors: Dr. Daniel Romero Nieto and Arne Lindbråthen (NTNU)

Project proposals from Associate Professor Liyuan Deng, *deng@nt.ntnu.no*

50 Nanocomposite membrane in a membrane contactor for CO_2 capture

Membrane based CO_2 capture is a promising technology for CO_2 emission control. Membrane contactor is a hybrid technology which combines the advantages of membrane separation with those of chemical absorption. Membrane in a gas-liquid contactor acts as a non-dispersive interface between the two fluid phases and its high specific surface area results in a compact system. The membrane in a contactor is not necessary to be selective but must be highly permeable or with high porosity. However, wetting and bubbling are critical drawbacks in porous membranes.

The objective of this work is to produce a nanocomposite dense membrane for application in a membrane contactor. The scope of the project will cover the following points:

(1) Preparation of a defect free, highly CO_2 permeable nanocomposite membrane containing carbon nanotubes (CNTs) and cellulose-based nanofibers.
(2) Permeability and selectivity test of the membrane under humid conditions at low pressure and room temperature.
(3) Characterization of the membrane: Morphology, chemical/thermal properties.

Supervisor: Ass. Prof. Liyuan Deng, Co-supervisor: PhD-student Muhammad Saeed

51 Supported ionic liquid membrane for high temperature CO_2 capture

In the past few years, the use of supported ionic liquid membranes (SILMs) for gas capture and separation has been widely studied because of its higher selectivity and better stability compared with conventional supported liquids membranes (SLMs). Most of the previous studies, porous polymeric membranes were used as support and thus limited the operation temperature of the membrane. Recently, ionic liquids with high CO_2 selectivity and excellent thermal stability are successfully synthesized in our group. This project will develop supported ionic liquid membranes (SILMs) using hydrophobic glass membrane as support for high temperature CO_2 capture. The main tasks are:

(1) Characterize the ionic liquids and the micro-porous glass membrane.
(2) Investigate the stability of both the flat-sheet and tubular supported ionic liquid membranes with different ionic liquids.
(3) Study the effects of temperature, permeate direction and the support structure on the gas permeability and selectivity.

Supervisor: Ass. Prof. Liyuan Deng, Co-supervisor: PhD-student Zhongde Dai

52 Evaluation of ionic liquids-based solvent for CO_2 absorption

Ionic liquids are attracting attention as a type of efficient and green CO_2 capture absorbents because of their distinctive properties such as negligible volatility, high CO_2 absorption capacity and reasonable thermal stability, with tailorable structure and property. As part of the 'MCIL-CO2' project (Novel Membrane contactor using ionic liquids for pre-combustion CO_2 capture), the properties of some selected task specific ionic liquids and their blends with low molecular polymers will be tested and optimized. The scope of the work includes:

(1) Synthesis of ionic liquids and NMR analysis
(2) Optimization of the blend composition
(3) Thermal stability test
(4) Physical properties of the solvent before and after CO_2 sorption.

Supervisor: Ass. Prof. Liyuan Deng, Co-supervisor: PhD-student Muhammad Usman

53 Investigation of solvent transport properties in a membrane

This is part of the 3GMC project on the development of a composite membrane (porous support coated with a thin dense layer) with suitable characteristics in terms of gas permeance and solvent compatibility, which can be used together with amine-based 3rd generation solvents for CO_2 absorption.
The scope of this specialization project is to investigate the transport properties of the thin dense layer with respect to the different absorbent solutions, both in terms of vapor permeability into the gas phase and of absorbent uptake within the polymeric matrix. The obtained results will be fundamental for the transport mechanisms of aqueous-amine solutions through the polymeric matrix, which can eventually be used to propose an empirical model to describe the permeability of absorbent solutions for various amines concentrations.
(A summer job position is in connection with this project)

Supervisor: Ass. Prof. Liyuan Deng, Co-supervisor: Postdoc Dr. Luca Ansaloni

54 Techno-economic study of pre-combustion CO_2 capture process using membrane process

Membrane-based CO_2 separation has become very attractive for more and more industrial applications, as it is environmentally friendly, energy-saving, easily scalable and require minimal maintenance. In the recent years Memfo group has developed and tested some highly efficient CO_2 separation membranes in lab scale, showing great potential for industrial applications.

This project intends to conduct a techno-economic study of a polymer membrane-based process for pre-combustion CO_2 capture. Hysis will be used to perform the simulation. The project scope includes:

(1) Evaluation and selection of membrane configurations and modules (e.g., flat sheet and hollow fiber) by process simulation.
(2) Design and optimization of multi membrane stages integrated with IGCC process with respect to energy consumption.
(3) Sensitivity analysis of the process on various operation parameters.
(4) Estimation and reduction of the capital cost and operation cost.

Supervisor: Assoc. Prof. Liyuan Deng, Co-supervisor: Prof. Magne Hillestad

Project proposal from Professor Magne Hillestad: *magne.hillestad@ntnu.no*

55 Autonomous Gas-to-Liquid process for off-shore production

We are developing a simplified process concept for a once-through gas-to-liquid conversion. Synthesis gas is produced through an air blown autothermal reformer (ATR) or alternatively with enriched air. The natural gas is pre-heated by the flue gas from a gas turbine. The synthesis gas from the ATR will be stoichiometrically hydrogen deficient. In parallel, and heat integrated with the ATR, hydrogen is produced through a heat exchange steam reformer, a high temperature water gas shift reactor and a membrane separation of CO_2 and hydrogen. The CO_2 rich gas is fed to the ATR which causes the hydrogen deficient syngas. The Fischer-Tropsch synthesis is staged with product withdrawal and hydrogen addition between the stages. This enables high conversion of syngas and high selectivity to higher hydrocarbons. The Fischer-Tropsch reactors are shell and tube fixed bed or microchannel fixed bed reactors. The unconverted syngas and surplus hydrogen will be used as fuel for the gas turbine. Detailed modelling of the fixed-bed reactor and process simulations are already under way, and the conversion of syngas can be higher than 90 %. The process concept will not contain an air separation unit. The FPSO will be autonomous, as it will be self-sufficient with power and water.

Tasks:

- Implement alternative kinetic models of the Fischer-Tropsch reactors
- Further development of the process concept; process and heat integration; utilization of surplus heat from the FT synthesis and other sources.
- Space requirements and optimization of reactor sizes, heat exchangers, gas turbine etc.

56 Nonlinear model predictive control of a CO_2 capture process

A dynamic model of a CO2 capture plant is developed and implemented in matlab. The model needs to be simplified and adapted to an NMPC environment, in this case Cybernetica Cenit.

Tasks

- Simplify the model without much loss of accuracy
- Implement the model in the programming language C.
- Design an objective function to be optimized for nonlinear model predictive control of load change and power price change

57 Modelling and optimization of a Biomass-to-Liquid process

A biomass-to-liquid plant consists of pretreatment, gasification , syngas cleaning and conditioning, Fischer-Tropsch (FT) synthesis, and products upgrading.

In the FT reactor the syngas is converted to liquid fuels on a cobolt (or iron) catalyst. There exist different reactor types of FT units, such as slurry bubble column, fixed bed and microchannel reactors. Here, we want to make a model of a fixed bed reactor of the FT synthesis in a new simulation system called VMGSim. A gasification model is already in the system.

- A kinetic model of the FT kinetics should be implemented in the simulation tool. This kinetic model takes into account a limited number of components, both alkanes and alkenes, and the selectivity to different products depends on composition and temperature.
- New process configuration of the BtL plant will be evaluated.

58 A solar thermal process for conversion of CO_2 and water to Fischer-Tropsch products

With solar energy it is possible to convert water or CO_2 to other products by using oxides at high temperatures. First, oxygen is expelled from the oxide at temperatures in the 1200 -1500 ^oC range. Then the oxide is exposed to water (or CO2) and the material will pick up the missing oxygen, thus yielding H_2 or CO. Subsequently, the hydrogen is reacted with CO_2 to give synthesis gas. The task is to optimize the process design and perform techno-economic modelling of a process making syngas for Fischer-Tropsch synthesis.
Cosupervisor: Erling Rytter

59 A solar thermal reactor model for splitting water or CO_2

With solar energy it is possible to convert water or CO_2 to other products by using oxides at high temperatures. First, oxygen is expelled from the oxide at temperatures in the 1200 -1500 ^oC range. Then the oxide is exposed to water or CO2 and the material will pick up the missing oxygen, thus yielding H_2 or CO. The reactor will operate in a swing mode between sweeping out oxygen and the reaction. The task is to create a dynamic model for continuous operation of the reactor.
Cosupervisor: Erling Rytter

Project proposal from Professor Hugo Jakobsen: *hugo.jakobsen@ntnu.no*

Background:

The reactor modeling group is involved in three centers for research based innovation (i.e., Senter for forskningsbasert innovasjon (SFI)) at the faculty (two of them at IKP), one of them is related to industrial catalysis and innovation (iCSI), a second one in subsea production and processing (SUBPRO), and a third one in metal production (MP) in material technology. In the SFI on catalysis the reactor modeling group will model the performance of chemical reactors considering chemical processes and transport phenomena in the reactor and pellets. Various forms of steam methane reforming, methanol production among other processes including carbon formation (metal dusting) might be considered. In the second SFI the reactor modeling group will focus on phase separation subsea. That is, separation of oil droplets in water, water droplets in oil or gas bubbles in water or oil. In this work the population balance equation is central and emphasis will be placed on examination of mechanisms and novel models for the fluid and solid particle breakage and coalescence at atmospheric and elevated pressures. In the third SFI on metal production (i.e., Silicon (Si) refining) very similar processes will be considered but a main difference is related to the very high temperature involved. In all projects strong collaborations with the collaborating experimental groups are required to provide empirical information for understanding physical

phenomena, model validation and parameter fitting. There is also some overlap between the different activities as it is also important to understand particle coalescence and breakage in multiphase reactors, and metal production to determine the interfacial area and thus the mass, heat and momentum transfer fluxes. Fluid flow and chemical reaction might also take place in all tasks. Common for all these modeling activities are also the use or development of stable, accurate, robust and efficient numerical methods for solving the model equations involved. The proposed projects are therefore intended for students that want to learn more about the numerical methods that might be used for solving models relevant for the work in these SFIs. Moreover the understanding of research challenges, phenomena and mechanisms can also be performed using existing models made by previous students, and by extending these investigations. The students might also propose modifications in the suggested projects.

Projects:

60 Population balance breakage closure discrimination

Population balance equation (PBE) modeling is a very relevant task in multiphase reactor technology, phase separation, extraction, crystallization, nuclear technology, meteorology, etc.

In this project an existing code for solving the population balance equation should be used to evaluate a number of closures for bubble and droplet breakage and coalescence. This project is a continuation of a previous student project dealing with breakage kernels, thus a number of MATLAB functions for solving the kernel functions solely are already available and documented in a review paper. The natural first step in this project is to verify the existing codes and the theory given in the review paper. A few new breakage kernel functions have been published during the last year or so, these should be included in the kernel function comparison as well. The next step is to compare the results produced by these kernel function closures when being a part of the population balance model solution. That is, both the MATLAB code for solving the whole population balance model and for many of the underlying breakage kernel functions exist and most of the work relates to the simulation of the predicted results without much coding. The predicted results should be compared to experimental data (from the literature or data measured at our own lab) for validation and kernel function discrimination.

Collaboration between the project 1 and 2 might be very useful.

Co- Supervisor: Post doc Jannike Solsvik

61 Population balance coalescence closure discrimination

Population balance equation (PBE) modeling is a very relevant task in multiphase reactor technology, phase separation, extraction, crystallization, nuclear technology, meteorology, etc.

In this project an existing code for solving the population balance equation should be used to evaluate a number of closures for bubble and droplet coalescence. This project is a continuation of a previous student project dealing with breakage kernels, thus a few MATLAB functions for solving the kernel functions solely are already available and documented. The natural first step in this project is to verify theory given in the literature and coding the kernel functions for comparison. The next step is to compare the results produced by these kernel function closures when being a part of the population balance model solution. That is, both the MATLAB code for solving the whole population balance model and for many of the underlying breakage kernel functions exist and most of the work relates to the simulation of the predicted results without much coding. The predicted results should be

compared to experimental data (from the literature or data measured at our own lab) for validation and kernel function discrimination.
Collaboration between the project 1 and 2 might be very useful.
Co- Supervisor: Post doc Jannike Solsvik

62 Population balance solution using the cell method

Population balance equation (PBE) modeling is a very relevant task in multiphase reactor technology, phase separation, extraction, crystallization, nuclear technology, meteorology, etc. Many numerical methods have been proposed over the last 2-3 decades for solving the population balance equation for various applications. In the reactor modeling group several methods in the family of the weighted residual methods have been investigated during the last 10 years.
In this project another method, similar to the finite difference and finite volume methods, should be implemented and compared to the existing weighted residual method solvers already available in the group. The interesting parameters to compare is method complexity, simulation time and solution accuracy.
Introductory, very simple populations balance problems will be considered. Having some experience the student should deal with more advanced problems considering particle breakage and coalescence.
Co- Supervisor: Post doc Jannike Solsvik

63 hp-adaptive spectral-element solver in MATLAB

Solving reactor model equations (or models for other unit operations) by the spectral element method optimization of the simulation time and accuracy can be achieved by optimal distribution of the elements, choice of the number of elements and the order of the approximation within each element.
Introductory, the project will consist in understanding the theory behind the method. Then, the method should be implemented for a simple test case with analytical solution to verify the implementation. Finally, the method should be applied to a practical problem to optimize the solution of the model equations.
The reactor modeling group has been investigating this family of numerical methods called methods of weighted residuals for applications in reactor simulations for more than 10 years thus some experience and knowledge on the methods will be provided. Hence, we might start out reproducing results of a similar algorithm published by members of the group.
Co- Supervisor: Post doc Jannike Solsvik

64 Numerical simulation of steam methane reforming in packed bed.

In this project a steady-state packed bed pseudo-homogeneous model should be solved by the collocation method being a method in the family of weighted residual methods. The model equations for the packed bed reactor are similar to the models known from the reactor modeling course. The purpose of this work is to study the optimal solution strategy of this model by use of the orthogonal collocation method. The project represents a continuation of an earlier student project thus some codes and a report is available for a useful introduction to the problem. The model can be implemented in the programming language MATLAB.
Collaboration between the project 5 and 6 might be very useful.
Co- Supervisor: Post doc Jannike Solsvik

65 Dynamic model for steam methane reforming for investigation of carbon production

In this project a dynamic packed bed model should be solved by the collocation method being a method in the family of weighted residual methods. The model equations for the packed bed reactor is similar to the models known from the reactor modeling course, but this time another numerical method should be employed for solving the model equation and long terms dynamic simulations should be performed to study the carbon formation behavior. The model can be implemented in the programming language MATLAB.
Collaboration between the project 5 and 6 might be very useful.
Co- Supervisor: Post doc Jannike Solsvik

66 Convection dominated convection-diffusion reaction problems

Solving the dispersion reactor model equations consisting of convection, diffusion and reaction terms might be challenging for convection dominated systems because of large concentration gradients. In this project the spectral element method solution of the corresponding mass balance equations should be optimized with respect to the simulation time and accuracy. This might be achieved by optimal distribution of the elements, choice of the number of elements and the order of the approximation within each element.
Introductory, the project will consist in understanding the theory behind the method. Then, the method should be implemented for a simple test case with analytical solution to verify the implementation. Finally, the method should be applied to a practical problem to optimize the solution of the model equations. A plug flow reactor model for steam methane reforming might be a useful example but other examples can be used as well.
The reactor modeling group has been investigating this family of numerical methods called methods of weighted residuals for applications in reactor simulations for more than 10 years thus some experience and knowledge on the methods will be provided. Hence, we might start out reproducing results of a similar algorithm published by members of the group.
Co- Supervisor: Post doc Jannike Solsvik

67 Modelling/simulation of transport of micro-and nanoparticles and drugs in tissue

The main task is to model the transport of cytotoxic drugs in the blood vessels to tumours by use of the governing equations.
A literature has to be performed to get an overview on what has been done before. A model should be formulated based on reasonable simplifications. Model parameter values have to be determined from the literature. A solution strategy should be examined. If time allows, the model should be implemented in matlab and solved.

The project represents an interdisciplinary project between the St.Olavs hospital, Biomechanics Division at Department of Structural Engineering, Department of bio-Physics and Department of Chemical Engineering on a better method for cytotoxic drugs treatment of cancer patients.

68 Modelling/simulation of US mediated transport of micro-and nanoparticles and drugs in tissue

The main task is to model the transport of cytotoxic drugs in the blood vessels to tumours by use of the governing equations.
The natural transport of micro- and nanoparticles is due to diffusive mechanisms and is thus rather slow. A working hypothesis is that ultrasound mediated transport will be dominated by convective transport and will thus be much more effective. In this project the mechanisms of this US radiation force should be elucidated. First by a literature study. Then a model should be formulated and solved to prove this hypothesis might work before the hypothesis will be verified in mice and rats.

The project represents an interdisciplinary project between the St.Olavs hospital, Biomechanics Division at Department of Structural Engineering, Department of bio-Physics and Department of Chemical Engineering on a better method for cytotoxic drugs treatment of cancer patients.

69 Design of experimental equipment for fluid particle breakage investigations

Fluid particle breakage due to various mechanisms are affecting the size distribution in dispersions in chemical reactors, separators, pipelines and in nature. This will also affect the interfacial transport of mass and separation efficiency, etc. In the ongoing SFI named SUBPRO a novel equipment for performing single fluid particle breakage experiments should be designed and built. Based on a literature study the limitations and possible advantages of the existing apparatus should be revealed and examined. A discussion of possible improved apparatus designs should be made. The data interpretation algorithms should be examined. If time allows, a lab scale apparatus might be built and characterized.

TKP4550/TKP4551 PROSESS-SYSTEMTEKNIKK (PROCESS SYSTEMS ENGINEERING)

Coordinator: Sigurd Skogestad

Project proposal from Professor Sigurd Skogestad, *sigurd.skogestad@ntnu.no*

70 Robust implementation of optimal operation of LNG refrigeration cycles.

Co-advisor: Adriana Reyes Lua

Project Background:

Natural gas is a fast growing energy resource in most regions of the world. Liquefaction plays an important role in the distribution of natural gas to locations in which pipeline transportation is not available. Boil-off gas (BOG) is the natural gas that boils-off during the voyage of a liquefied natural gas (LNG) carrier. Pressure in the tanks cannot exceed a certain limit and the common way to avoid overpressure is to burn BOG to onboard power steam turbines, or simply flare it. Small-scale LNG plants have been installed recently on LNG carriers to re-liquefy BOG, reducing product loss and minimizing flaring.

As the majority of small LNG plants are either onboard carriers or in remote locations, specialized staff is not available and there might be limitations for obtaining continuous or reliable information regarding the process. For example, chromatography for refrigerant or natural gas composition is not readily available. This situation makes difficult to track changes in the process and to rely on onboard personnel to perform the appropriate adjustments every time a disturbance occurs.

The optimum composition of the refrigerant is determined by the natural gas feed composition and pressure, plant pressure, and ambient temperature. Ideally, refrigerant composition would be adjusted accordingly, but it is not a practical or even applicable solution.

Additionally, refrigerant may leak from the pipeline. As refrigerant components do not leak at the same rate, the composition of the refrigerant varies and the optimal operating point might also change. Being onboard a carrier, it is a challenge to maintain near to optimal operation when having this type of disturbances, which are in principle very difficult to measure directly.

This situation is an excellent example to explore the convenience of using self-optimizing control variables. The concept behind this is to maintain near-optimal (with acceptable loss) operation in presence of disturbances and implementation errors using constant set points (Skogestad 2000, 2004).

The analyzed plant would preferably be the one described by (Nekså et al. 2010) but it could be another simple LNG plant.

Proposed activities:

- Literature search on: small LNG technologies, types of models, and typical control strategies for this type of processes.
- Modeling for control purposes. There are two possible options:
  - Develop a steady state HYSYS model of the refrigeration cycle.
  - Develop a simple (possibly dynamic) model of the refrigeration cycle using MATLAB.
- Optimization: analysis of optimal operating conditions when disturbances occur.
- Analysis of research challenges. May include a proposal for Master thesis work.

Specific activities and methods will be discussed and defined with the project student. The student will write a project description at the beginning of the semester, specifying the actual objectives and proposing a time schedule.

References:

Nekså, P., E. Brendeng, M. Drescher, and B. Norberg. 2010. "Development and Analysis of a Natural Gas Reliquefaction Plant for Small Gas Carriers." *Journal of Natural Gas Science and Engineering* 2(2-3): 143–49. http://www.sciencedirect.com/science/article/pii/S1875510010000326 (January 20, 2015).
Skogestad, Sigurd. 2000. "Plantwide Control: The Search for the Self-Optimizing Control Structure." *Journal of Process Control* 10(5): 487–507. http://dx.doi.org/10.1016/S0959-1524(00)00023-8 (December 3, 2013).
———. 2004. "Near-Optimal Operation by Self-Optimizing Control: From Process Control to Marathon Running and Business Systems." *Computers & Chemical Engineering* 29(1): 127–37. http://www.sciencedirect.com/science/article/pii/S009813540400184X (October 3, 2014).

71 Optimization of the synthesis-gas loop as example for integrated processes.

Co-advisor: Julian Straus

Modern plants in the ammonia industry are highly integrated. This is on the one hand caused by the small equilibrium conversion in the gas phase synthesis reaction and on the other hand due to the strong competition in the market. Hence, energy recycling to utilize the heat of the reaction and compression efficiently and reactant recycling play a crucial role. Figure 1 provides and overview of the synthesis loop indicating the integrated structure.
This integration leads to problems in modelling using the traditional sequential-modular approach through the huge amount of iterations needed to solve the flowsheet and the associated computational costs, especially for nested recycle loops, (recycle loop within a recycle loop). Additionally, convergence is not always achieved. Hence, conventional optimization approaches are difficult to apply. Our idea to circumvent this problem is to develop a new approach by splitting the big model into smaller sub-models and simultaneously treating the inputs from the non-used sub-models either as disturbances or replace the sub-model itself with a simplified model, which can be linear or more advanced.
This core of this research project is hence to investigate the different possible approaches to define the simplified model and the influence of its properties on the optimization outcome:

1. Identification of state-of-the-art approaches to optimize integrated plants and familiarization with Aspen HYSYS steady state mode.
2. Mathematical definition of simplified models and programming in MATLAB.
3. Implementation of the models in HYSYS and analysis of their behavior.
4. Definition of challenges and opportunities for future research (*e.g.* for a M.Sc. thesis).

The complete steady state model of the synthesis loop is already existing in HYSYS and will be used as starting point. This project is part of an industrial cooperation with Yara.

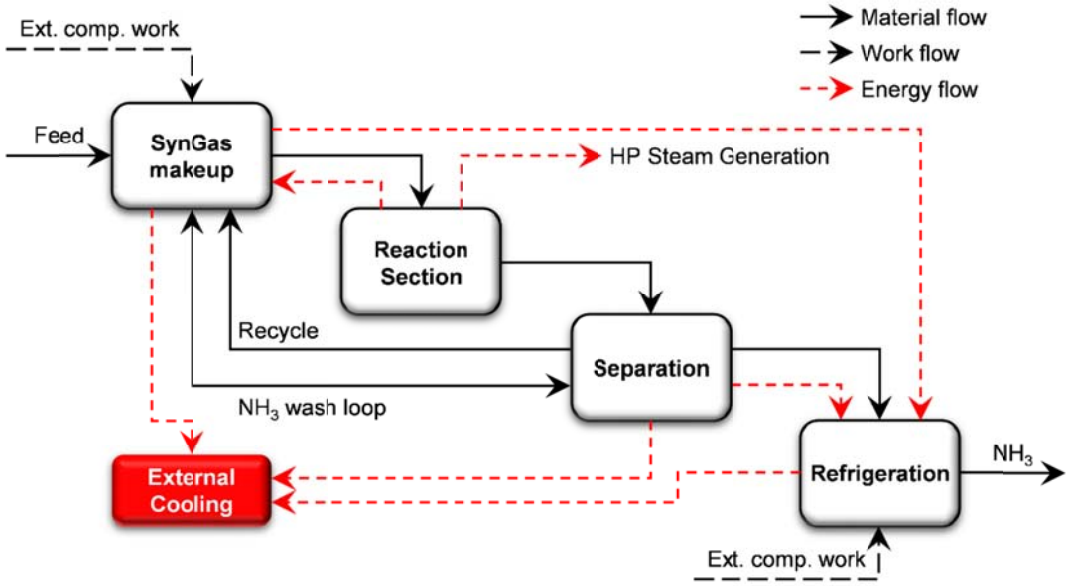


Figure 1: PFD for the synthesis loop of an arbitrary ammonia plant

72 Subsea processing. Co-advisor or main advisor: Johannes Jäschke

a. Subsea separation of oil and water;
b. Subsea water treatment.
c. Subsea separation of gas and liquid (oil)
d. Subsea boosting

The projects nr .. to … will include the following:

part 1. Industrial use (survey, first month)
part 2. Dynamic and steady state models (survey, second month)
part 3. Control strategies (survey, third month)
part 4. Research challenges and proposed research (may include a proposal for Master thesis work.)

73 Industrial use of condition monitoring of process and equipment variables, a survey with emphasis on the oil and gas industries,

Co supervisor: Johannes Jäschke

74 Case study at Perstorp Co. Advisor: Prof. Krister Forsman

Project proposals from associate professor Johannes Jäschke: *jaschke@ntnu.no*

Category 1: General topics

75 Chance-constrained optimization. A survey and small examples highlighting potential and challenges for use in model predictive control.

When optimizing process plants under uncertainty, it is sometimes desired that certain variables satisfy operational constraints for "most of the time". This can be translated into the mathematical requirement that the constraint is satisfied with a given probability, e.g. 95%. Such optimization problems, where the constraints are required to be satisfied with a given probability are called "Chance-constrained optimization problems"
The goal of this project is to gain an initial overview over chance constrained optimization and solution approaches for such problems.
This challenging project requires ability to work independently, good knowledge in numerical optimization (e.g. TTK4135 Optimization and Control), and keen interest in learning more about optimization.
Tasks:

1. Survey: basics and solution methods for chance-constrained optimization problems
2. Toy examples for demonstration purposes
3. Survey: Application to model predictive control
4. Research challenges and proposed research (may include a proposal for Master thesis work.)

Category 2: Modelling and monitoring compact separation equipment

The task of these projects is to develop simple models of compact gas-liquid separators that are suitable for optimization and control.
In order to be able to produce hydrocarbons economically from reservoirs under difficult circumstances, such as ultra-deepwater conditions or low reservoir pressure, is necessary to separate oil, gas, and water at the sea floor. This subsea separation enables efficient and economic transport over long distances, and also reduces the back pressure on the reservoir, which leads to increased production.
For economic reasons, the separators used subsea are built very compactly, and this comes with unique operational challenges. These compact processes are often very coupled, and due to the relatively small dimensions, they exhibit fast dynamics, which are challenging when controlling the processes.
Moreover, these models can be used to monitor the process and the equipment of equipment that is difficult to access.
We are looking for someone who likes to program in matlab or a similar language, with good mathematical skills the ability to work independently.

76 Modelling of compact gas-liquid separators

Tasks:

1. Industrial use (survey, first month)
2. Dynamic and steady state models (survey, second month)
3. Control strategies (survey, third month)
4. Research challenges and proposed research (may include a proposal for Master thesis work.)

Supervisor: Associate Professor Johannes Jäschke and Professor Skogestad

77 Modelling of compact liquid-liquid separators

Tasks:

5. Industrial use (survey, first month)
6. Dynamic and steady state models (survey, second month)
7. Control strategies (survey, third month)
8. Research challenges and proposed research (may include a proposal for Master thesis work.)

Supervisor: Associate Professor Johannes Jäschke and Professor Skogestad

78 Industrial use of condition monitoring of process and equipment variables, a survey with emphasis on the oil and gas industries

Tasks:

1. Industrial use (survey, first month)
2. Dynamic and steady state models (survey, second month)
3. Control strategies (survey, third month)
4. Research challenges and proposed research (may include a proposal for Master thesis work.)

Supervisor: Associate Professor Johannes Jäschke and Professor Skogestad

Category 3: Projects in collaboration with DNV GL in Høvik

Note that there may be summer jobs possible. Please mail the contact at DNV GL below.

79 Modelling of multiphase flows in subsea separators

Background

The subsea sector has a great improvement potential with regards to employing new technology. However, the sector is conservative because of the risk related to the uncertainties that relies in the difficult access for doing repair and maintenance subsea. The present work focuses on methods for qualification of subsea processes and seeks to give guidance to the subsea sector for applying new technology with the required confidence for subsea use. The main motivation is to create improved and more cost-efficient methods for subsea process technology qualification.

Objective

Investigate for gas-liquid separation processes relevant for “subsea factories” the potential coupling between fundamental physical and chemical processes at micro scales and failure modes at the macro level.

- ***Scope of work***

1. Literature review of multiphase flows and subsea separation processes, including modelling in general and state-of-the art in multi-scale modelling in particular.
2. Identify, select and describe a relevant subsea separator case study
3. Identify and discuss potential failure modes (risks) that is related to the coupling between fundamental physical and chemical processes and the equipment in multiphase separator flow
4. Review and discuss relevant models to model and simulate the identified failure modes of concern. Discuss pros and cons of the various models and use this to conclude and select model.
5. Develop model for one or more selected process-equipment failure mode.
6. Develop a multi-scale model for one or more failure mode and compare with other model identified in pt. 4 above. Compare results with experimental data from case study in pt. 2 above.

- ***Deliverable*** Project report

- ***Summer job***

There might be a possibility for summer job financed by DNV GL. Contact Frank Børre Pedersen, Program Director, Oil & Gas and Energy Systems in DNV GL Strategic Research and Innovation, for more information. Email:Frank.Borre.Pedersen@dnvgl.com.
Work place: Høvik.

Advisors:
Supervisor: Johannes Jäschke, Associate Professor, NTNU
Co-advisor: Tore Myhrvold, DNV GL
Co-advisor: Andreas Hafver, DNV GL

80 Condition and performance monitoring of subsea systems

Background
Subsea installations are remote by nature and intervention is much more difficult and costly. This makes it important to design robust and failure tolerant components and systems, and to develop solutions and strategies for on-line condition and process monitoring and for robust control.

Condition and performance monitoring (CPM) becomes increasingly challenging for complete subsea production and processing systems because of the increasing amount of generated data, especially if rotating equipment is installed.
Bayesian Networks (BN) have previously demonstrated favourable capabilities for online process monitoring in chemical processes, but it seems not so far to have been in use for subsea systems.

Objective
Investigate the applicability of Bayesian Networks for condition and performance monitoring of subsea process systems.

Scope of work

1. Literature review of
    a. Subsea process systems and subsea process monitoring and control, including "All subsea systems" such as Statoil's subsea factory concept.
    b. Previous work (state-of-the-art) in application of Bayesian Networks as a tool for process monitoring
    c. Investigate knowledge transfer potential for CPM from other industries (such as in maritime and aviation) to the subsea industry
2. Review and discuss pros and cons of using BN compared to other methods for process monitoring and control to conclude on the applicability of BN.
3. Investigate applicability and discuss pros and cons of coupling of BN solvers with process modelling and simulation tools
4. Demonstrate by a case study the use of BN for process monitoring

Deliverable Project report

Summer job There might be a possibility for summer job financed by DNV GL. Contact Frank Børre Pedersen, Program Director, Oil & Gas and Energy Systems in DNV GL Strategic Research and Innovation, for more information.
Email:Frank.Borre.Pedersen@dnvgl.com. Work place: Høvik.

Advisors:
Supervisor: Johannes Jäschke, Associate Professor, NTNU
Co-advisor: Tore Myhrvold, DNV GL

81 Subsea Integrated Operations

Background
Over the past 15 years, subsea technology has moved from subsea wells, manifolds, flowlines, and templates, to include subsea boosting, separation and now compression. Some oil companies and subsea suppliers are targeting moving ever-larger sections of the topside subsea. Without direct access to the subsea installation the operator must rely on sensor data, management and analyses of large amounts of data.

Integrated Operations (IO) is the integration of people, organizations, work processes and information technology to make smarter decisions. IO is enabled by global access to real-time information, collaborative technology and integration of multiple expertises across disciplines, organizations and geographical locations.

Objective
Harvest knowledge from research done at the Center for Integrated Operations (http://www.iocenter.no) and how this can be applied for a subsea process system.

Scope of work
1. Literature review of:

- Subsea processing systems, for instance consisting of multiphase pumps, separators, and compressors with specific focus on the operational phase.
- Integrated Operations, both research done at NTNU IO Center and others.
- Describe in more detail what research done at NTNU IO center is relevant for a subsea processing station.
- Identify and discuss main drivers/barriers for Integrated Operations.

2. Select one of the relevant research areas and describe how this can be implemented for a subsea system.
3. Identify, select and describe a relevant subsea process case study:
   a. Set up a process model for the system (Hysys).
   b. Identify what sensor/controls that is needed as a minimum
   c. Describe how IO will affect the design and infrastructure of the process system.
   d. How will the implementation of IO affect the people/organization and decision making for an operator

Deliverable

Project report

Summer job

There might be a possibility for summer job financed by DNV GL. Contact Frank Børre Pedersen, Program Director, Oil & Gas and Energy Systems in DNV GL Strategic Research and Innovation, for more information. Email:Frank.Borre.Pedersen@dnvgl.com.
Work place: Høvik.

Advisors

Supervisor: Johannes Jäschke, Associate Professor, NTNU
Co-advisor: Øystein Grande, DNV GL

82 Subsea process system qualification

Background

For subsea process systems, there is a need to develop and qualify the necessary technology elements, processes, and sub systems enabling the entire system to function as intended over its lifetime. System qualification is a collaborative task, including process, power & control. Current process technology qualification approaches have equipment focus. Subsea process qualification need more focus on the physical and chemical processes and integration with interfaces to equipment, power and control (system qualification).

Objective

Develop knowledge and methods in subsea process technology qualification and subsea system qualification.

Scope of work

4. Literature review of:
   - Subsea processing systems, for instance consisting of multiphase pumps, separators, etc. with specific focus on the control systems and interfaces to process and power
   - Technology qualification in general, for instance DNV-RP-A203, API-RP-17n or similar

- Subsea industry's state-of-the-art methods for qualification of subsea control systems and qualification of interfaces between control and process and power in a subsea processing system

5. Identify and discuss one or more system failure modes related to process-control interfaces
6. Identify and discuss pros and cons of potential methods for qualifying the identified failure mode(s), e.g. mathematical model, experiment, etc. to conclude on the applicability of the various methods
7. Develop a model for one or more of the identified system failure mode(s), carry out simulation of potential scenarios and report uncertainty in the results in order to demonstrate qualification.

Deliverable

Project report

Summer job

There might be a possibility for summer job financed by DNV GL. Contact Frank Børre Pedersen, Program Director, Oil & Gas and Energy Systems in DNV GL Strategic Research and Innovation, for more information. Email:Frank.Borre.Pedersen@dnvgl.com.
Work place: Høvik.

Advisors:

Supervisor: Johannes Jäschke, Associate Professor, NTNU
Co-advisor: Tore Myhrvold, DNV GL

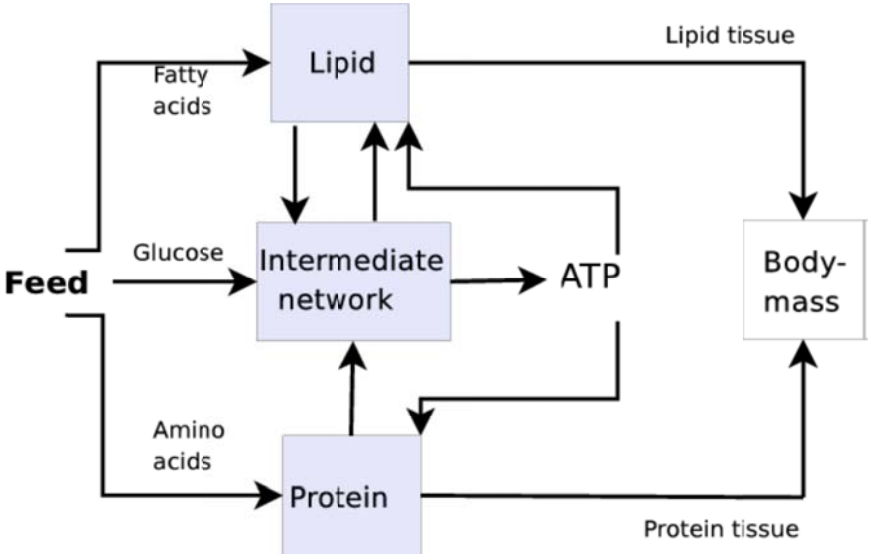
Project proposals from Associate Professor Nadav S. Bar, *nadi.bar@ntnu.no*

83 Simulation and numerical optimization of a dynamic model of growth (System biology: applied modeling)

A novel model that predicts the growth of fish, given the feed type and environmental conditions, has been developed during 2003-2009. The model traces the nutrients, proteins and fat, through the metabolic processes of the body, and basically it is a set of ordinary differential equations. It was implemented in Matlab code, using a constant time step, first order Euler integration method to solve the differential equations.

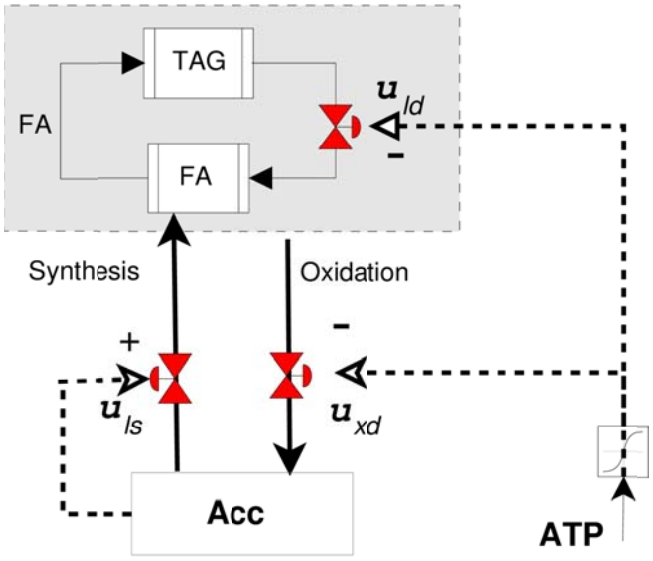
However, this method for solving the differential equations is very inefficient, and a more practical implementation is needed.

The main goal of this project is to optimize the integration method of the model, using a combination between a constant time-step and Matlab's ODE time variable solvers (ode45, ode15s). The project is interesting since it

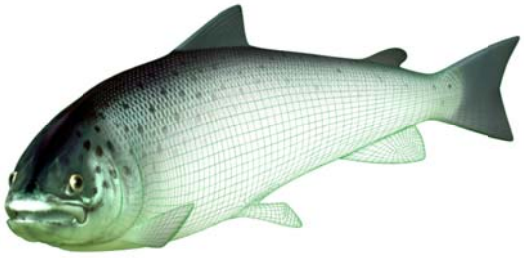


attempts to give a practical, industrial, applied solution to a theoretical model. If the program (the implementation of the model) could be optimized and made efficient, it will have a great value to the aquaculture field, both in study fish development and design more healthy fish feed.

The candidate will gain many useful skills, that are very important in the research and development in industry, such as how to make model solvers more efficient, how to simulate and solve models using ordinary differential equations, a very important aspect of any applied modeling.



Main Supervisor: Assoc. Professor Nadav S. Bar
Collaboration: Assoc. Professor Johannes Jaschke



84 Modeling and simulations of bat flight and sonar in 3dimensions (Systems biology: Neuroscience).

It was found in 2010 (Science Magazine, Yovel et al. 2010) that Egyptian fruit bats apply a sonar measurement strategy that is similar to the strategy used by certain GPS. One of the explanations was that the bat tries to reduce the sonar measurement noise during its flight to the target (which can be fruit or insect).

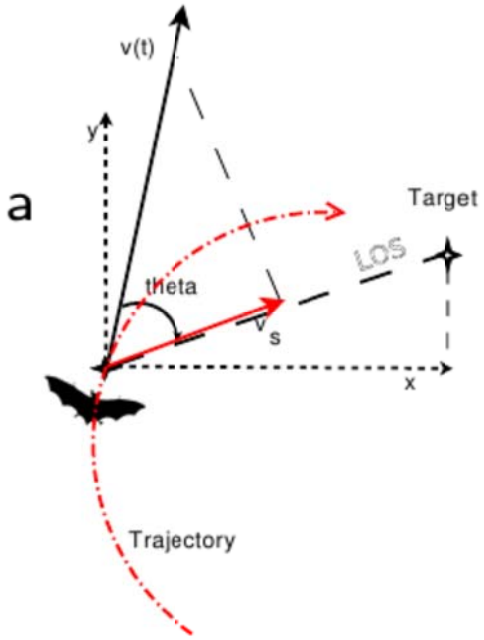
In our lab (in cooperation with Univ. of Maryland, Weizmann Institute of Science, and the U.S. defence), we developed a dynamic model that estimates the x-y trajectories of the bat's flight as it converges to its target, and explored the strategies it applies to reduce the noise that is reflected from the surroundings (trees, leaves, and other objects around the target). We found that the bat's brain processes the sonar information and filter the noise in a very interesting manner, stems from the fact that the bats has to apply a specific flight control system due to its non-linear flight maneuvers.

The main goal of the project is understand the sensory system of the bat, understand the strategies it uses for navigation, both long distance and short. We would like to analyse the data about the navigaion using earth's magnetic field we collected from Mexico.

The project can be later integrated in Master thesis, studying the sonar effect and the flight convergence strategies.

See Schrødinger's Katt, NRK, 19.mars 2015.

Main Supervisor: Associate Professor Nadav S. Bar



85 Modeling and simulation of path finding and tracking, applied to ants

Most of the ants navigate their way in the path, by sensing of pheromones, for the nest to the target (food) and back, by sensing the pheromones that creates the path using two antennas. However, the manner they are doing so is still unknown. We have gathered data, using manipulation of the trail width and the strength of the pheromone, which indicate that the ants do not walk where the smell is strongest, but walk more to the side of the trail. We believe that the ants uses a special form for simple optimization to sense its location, and process in in its simple brain to calculate its direction.

The student who will choose this work will join the intenational group of researchers, and his/her part will be to model and simulate the path-finding algorithm that we believe the ants use. The modeling will be in matlab, and will include very simple optimization strategies. Successful completion of the project/ diplom will result in a publication in a high impact international journal.

Sounds interesting? More details? Contact Nadi.bar@ntnu.no.

86 Development of appetite model

The reasons of why and when we are hungry is not well understood. The marked is 'flooded' with magic solutions to suppress appetite and loose weight, non were proven satisfactory.

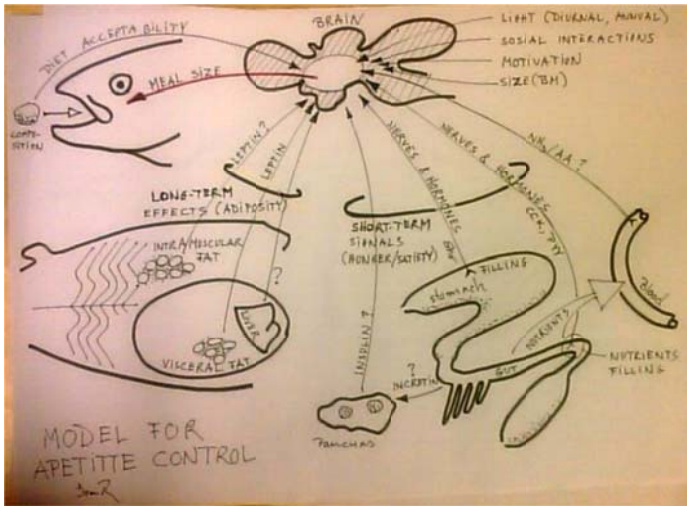
In aquaculture, appetite is the limiting stage for the growth of fish. We wish to understand why, and when, the fish has an increased appetite. For that, we will create a dynamic model of appetite with the information we have both internal and external factors (see Figure below). Many factors and relationships that affect appetite are already known but is not structured in to one system.

The main purpose of the project is to map the factors that affect appetite and feed intake, and structure them in a qualitative model. The task will be to group all these known factors in a systematic manner. These factors forms the states of the system, that is, the minimum set of characteristic variables that gives an adequate representation of the system.

The modeling process itself involves putting together some of the important states and their relationships into one integrated simple model by using differential equations.

The student will use programming language such as matlab, to apply the differential equations and to simulate the system. No previous biological knowledge is required. It is desired to continue the project to a master thesis. Job possibilities are promising, both in Trondheim (Biomar), stavanger, oslo and more (Marine harvest, Ewos, and more).

Main supervisor: Asoc. Prof. Nadav S. Bar



Project proposals from Professor Heinz Preisig, *heinz.preisig@ntnu.no*

The projects are in no specific order. Projects are offered both as "fordypningsprosjekter" and master projects. Level changes accordingly. If you have a pet project not listed - we can discuss it.

87 Overseas cooperation: Nonlinear frequency analysis

Literature is scarce in this domain as frequency analysis is often thought to be limited to linear systems. There are however techniques and classes of models for which nonlinear frequency analysis is applicable.
This project is of joint interest with Andreas Linninger professor in the Bioengineering department at University of Illinois at Chicago, Chicago, IL. So this could imply that one organises a stay at Chicago.
Supervisor and daily contact: Heinz A Preisig

88 Overseas cooperation: Model of a rat

Medical technology has come a long way in terms of the ability to measure blood flow, vessel distribution and the physical properties of living tissue. In collaboration with Andreas Linninger professor in the Bioengineering department at University of Illinois at Chicago, Chicago, IL, we want to map a well-documented species into a network description that describes the blood flow in the body, including all organs, which we then plan to extend with simple models for the metabolisms in the different organs.
This project is of joint interest with Andreas Linninger professor in the Bioengineering department at University of Illinois at Chicago, Chicago, IL. So this could imply that one organises a stay at Chicago.
Supervisor and daily contact: Heinz A Preisig

89 CFD: Temperature distribution in milli-reactor, CFD-simulations

FluiTec is a small, hi-tech company located in Switzerland who is the innovator of a new reactor concept called ContiPlant. It is a Lego-like idea in which milli-reactors are the building blocks. These reactor types are currently tested by the large polymer industries to construct small-scale productions that can be placed into containers and thus are mobile. Production range is in the 10 k tons per year.
An expert group has constructed a rig and we have had a master project joint with BASF doing CFD calculations towards the simulation of these reactors for polymer systems. This was done with the main research division of BASF that looks into new production technologies.
So we have now one of a four university installations of the reactor, which was provided by the producer FluiTec. Our installation is equipped with a cutting edge temperature sensor which is based on an optical laser-inferential meter to measure temperatures along the axis of the reactor on 8 positions with only one fibre. The fibre is less than in the order of 0.2 mm and the reactor inside approx 6 mm. So we are talking very highly sophisticated reactor equipment with highly sophisticated measurement equipment. We shall aim at constructing a dynamic residence-time distribution experiment for research and felles lab and using CFD to simulate the behaviour of the plant on a large computer, possibly NTNU's supercomputer.
Supervisor and daily contact: Heinz A Preisig

90 CFD: Residence-time distribution in various mixed systems, CFD simulations

As part of the renewal of the felles lab, I am extending the scope of reactor-engineering related projects. In particular the concept of residence-time distribution is being one of the targets. We have built two flexible bench-scale experiment, which demonstrates the hydraulic behaviour of various different physical systems. We constructed new conductivity sensors which we are implementing and testing. We would now like to model the sensor - injection manifold using OpenFoam CFD simulation with the objective to better undserstand their behaviour and check and if necessary improve the design of the injector and the sensor.
Supervisor and daily contact: Heinz A Preisig

91 Multi-scale modelling: Design of input patterns for computational experiments

Multi-scale modelling is a key to integrate nano-models into macroscopic descriptions. On a given scale, models of the lower scale are integrated by making time-scale and length-scale assumptions. If the scale difference goes over the limit particular processes / continuous processes, this involves a population averaging whilst retaining conservation of the fundamental physical quantities. On the upper scale, the behaviour of the lower scale is captured in a surrogate model, thus a model that replaces the detailed lower-scale model. This surrogate model is based on the length and time scale assumptions. Its key feature is simplicity in the sense of low computational complexity. As it is integrated to represent the lower scale these surrogate models are often in the most inner loop of the computation and thus very frequently evaluated making the need for low computational complexity evident. We would choose a particular toy problem from the EC project MoDeNa, which is on multi-scale modelling of polyurethane foams from quantum to mechanical properties. The lower scale is then the experiment and we inject conditions for the lower scale such that we optimise the information contents of the input/output signals in the context of the surrogate model. Common criterion is thus the Fisher information matrix, which gives a measure of the minimal variance bound of the estimate. This is then minimised by changing the conditions. The mathematical problem finds more than one formulation. The common one is to use a linearised approach but in many cases the problem is strongly nonlinear and should be handled using nonlinear optimisation. Constraint is then the surrogate model and in some cases also hard constraints on the conditions due to validity limitations of the involved models.
MoDeNa link: http://modenaproject.eu/
Supervisor : Heinz A Preisig, MoDeNa team.

92 Modelling fundamentals: Ontology for material models

Models representation overt the scales and link to experiments. This work is also associated with the EC project, but aims at a wider objective to define standards for models and associated data.
The material communities are more and more able to predict the behaviour of materials. Multi-scale modelling is a key to integrate nano-models into macroscopic descriptions. On each scale assumptions are being made about the lower scale and thus a hierarchical system of models is constructed that eventually provides a description of the material or process on the production scale. On all levels, models are being generated and all models are an integrated part of the overall description. If one wants to use these models for the manipulation of the quality of the product, then one could talk of control. If one uses the

models for getting alternative products, then one would talk about product design, if one uses them for design, then it is plant design and if it is for operations than it is mostly control. In all cases the "control" aspect is important.
Currently models and software are intimately linked together, well in most cases they form a monolith on the respective scale and it is re-implemented for each and every application of the model. This is what we should change: models should be in a library in a generic form, such that we can take them out, compile and integrate them with the solver code and generate stand-alone, special purpose computational tasks. In order to be able to do so, the models have to be made available in a generic form. This form must be suitable to capture essentially any of our models and be stored in a form that makes it easy to translate them into any kind of target code. Software factories come to mind, but also model reduction and simplification procedures.
MoDeNa link: http://modenaproject.eu/
Supervisor Heinz A Preisig, MoDeNa team.

93 Green chemistry, SINTEF cooperation: SINTEF Bio-Refinery

Humans have to integrate better into the earth's biotope. Mining of carbon in the form of oil, gas and coal, is not sustainable and has many undesired effects on the earth's climate. Future generations will have to be more conscientious about the environment on a global basis
Supervisor: Heinz A Preisig and possibly SINTEF

94 Felles lab: Continuous distillation

We have now four working distillation columns in the felles lab. All of them use an industrial configuration.
What we like to do is to improve all by adding workable pressure measurements in the boiler so as to measure the level. Two columns should be extended to continuous columns. This implies that we refurbish two columns with additional pumps to enable them running in continuous mode. we have now the ability to build the pumps ourself so as to have superior performance over commercial pumps. We combine an advanced pump head with an advanced motor, both from different companies.
Effort focus can vary from control, software to more engineering-type activities.
Supervisor and daily contact: Heinz A Preisig

95 Modelling-fundamentals & tooling: Computer-aided modelling

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

Recent publication: http://dx.doi.org/10.1016/j.compchemeng.2010.02.023 being noted as one of the most cited papers of Comp & Chem Eng in the period 2010-2013
An excellent opportunity to learn more about modelling and if so desired, programming.
Supervisor and daily contact: Heinz A Preisig

96 Felles-lab: Control and Felles lab rejuvenation

We have now completed the main effort of re-building the felles lab, but would like to extend further so as to make it more versatile and more flexible. There is also an ongoing discussion of extending the scope of the lab to other courses. Also 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.
An excellent opportunity to learn about real-time programming, control and making experiments fool proof.
Supervisor and daily contact: Heinz A Preisig

97 Process design: Automatic Safety and Hazard Analysis

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. Possible co-operation with SINTEF on hydrogen gas fuel stations or the like.
Supervisor and daily contact: Heinz A Preisig

98 Modelling - tooling: Simple Thermo Server

The Process Systems Engineering group is heavily involved in process modelling particularly distillation. Distillation models and associated material models are used at a high frequency.
The project is aiming at implementing a server that provides:

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

The material model software is running and we are using it in a variety of ways. We thought it would be fun and very useful to build a little user interface that enables the interactive use of what the core can generate. This could then be put on-line in the form of a web page, for example. We have a rather generic distillation column model that is quite generally parameterised, which could be augmented with an appropriate interface to make it usable on the web.
Such a system has been realised for Yara. A prototype sever exists and is currently operable for ammonia, nitric acid and urea production. The Matlab interface is already working and we are working on an interface to other computer languages such as Python.
Supervisors: Heinz A Preisig, Tore Haug-Warberg

99 Modelling fundamentals: On time scaling in chemical processes

The Process Systems Engineering group is heavily involved in process modelling. The objective is to generate a very general framework in which models for the process industry can be generated quickly and rapidly.

Making time-scale assumptions is done very frequently in the modelling process. Mostly it is not really done explicitly, but just kind of happens. Examples are decision on how to model a heat transfer, for example using an overall heat transfer model is making a time-scale assumption about the distributed transfer system to be of negligible capacity. Similar assumptions appear all over the place and we would like to put this problem into a more systematic framework.

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

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

100 Process & experiment: Process Identification using Wavelets

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

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

Supervisor and daily contact: Heinz A Preisig

TKP4560/TKP4561 BIORAFFINERI – OG FIBERTEKNOLOGI (BIORAFFINERY AND FIBRETECHNOLOGY)

Coordinator: Associate professor Størker Moe

Project proposal from Professor Øyvind W. Gregersen,
oyvind.gregersen@ntnu.no

101 CNF-CNF Hydrogels as Bone Tissue Scaffolds

Cellulose based hydrogels are being investigated as bone tissue scaffolds in collaboration with the University of Bergen (UiB). Cell-scaffold interactions are highly dependent on the choice of material, both with respect to their surface chemistry and mechanical properties. This project proposal aims at producing hydrogels containing various amounts of crystalline (CNC) cellulose in an amorphous cellulose (CNF) network, in order to tailor gel properties to optimize bone cell compatibility. This is an iterative process, where a range of mechanical, electron and atomic force microscopy characterization methods will be applied on the hydrogel at NTNU, before hydrogel fabrication and design parameters are evaluated by investigating cell-scaffold interactions at UiB.
Techniques: Rheometry, electron microscopy, microindentation, AFM.
Relevant for: Chemists, biochemists, nanotechnologists, biophysicists and material scientists.
Supervisor: Kristin Syverud, Professor II, kristin.syverud@pfi.no
Co-supervisor: Jonathan Torstensen, Ph. D. candidate, jonathan.o.torstensen@ntnu.no
Ahmad Rashad, Ph. D. candidate (UiB), dr.arashad@gmail.com

102 Modelling Gas Permeability in Nanocellulose based materials

Nanocellulose based materials have applications in membrane and packaging technology. Gas and ion permeabilities in these materials depend on material structure and -constituents. The goal is to model transport of oxygen in/through a nanocellulose film and carbon dioxide and bicarbonate in/through a nanocellulose/polymer membrane. Modelling will be done based on available experimental data and transport theory. The developed models will serve to improve both material design and to examine transport hypothesis.
Techniques: Modelling in MatLab, Phyton, C++
Relevant for: Computer scientists, chemists, biochemists, biophysicists, nanotechnologists, material scientists.
Supervisor: Øyvind W. Gregersen, Professor, oyvind.w.gregersen@ntnu.no
Magne Hillestad, Professor, magne.hillestad@ntnu.no
Co-supervisors: Vegar Ottesen, Ph.D. candidate, vegar.ottesen@ntnu.no
Jonathan Torstensen, Ph.D. candidate, jonathan.torstensen@ntnu.no

103 Fluorescence-Based Characterization of Nanocellulose Materials

Nanocellulose as a material is highly hydrophilic. Interactions with water are of importance for products associated with the material, and means to characterize the material in various states of wetness are therefore of importance scientifically and industrially. While several such techniques have been used on wood fibres and other large cellulose fibers there are very

few examples of application of optical techniques to study nanocellulose. The general idea is to develop protocols for applying these techniques on nanocellulose composites and hydrogels.
Secondly, these techniques are to be used to study a broad range of nanocellulose properties, such as swelling and molecular interactions.
Techniques: Fluorescent staining and fluorescence microscopy techniques: CLSM, SHG, STED, FRET
Relevant for: biochemists, biophysicists, nanotechnologists, material scientists
Supervisor: Øyvind W. Gregersen, Professor, oyvind.w.gregersen@ntnu.no
Co-supervisors: Vegar Ottesen, Ph.D. candidate, vegar.ottesen@ntnu.no
Jonathan Torstensen, Ph.D. candidate, jonathan.torstensen@ntnu.no

104 Hydrophobic Thin Films

Films of nanocellulose have excellent gas barrier properties, are transparent, strong, flexible, non-toxic and biodegradable. However key properties such as the gas barrier and strength are compromised when exposed to water in liquid or vapor form. The protection of the cellulosic material is therefore crucial. In this project the candidate will be working on the development of a thin-film coating which protects the nanocellulose from water vapor and liquid water on a short term. The goal is to produce a flexible cross-linked hydrophobic thin-film coating covalently bound to the nanocellulose film.
Techniques: Gas transmission measurement techniques, FTIR, mechanical testing techniques
Relevant for: Chemists, material scientists, nanotechnologists
Supervisor: Øyvind Weiby Gregersen, Professor, oyvind.w.gregersen@ntnu.no
Co-supervisor: Vegar Ottesen, Ph.D. candidate, vegar.ottesen@ntnu.no

105 3D FIB/SEM and STEM Nanocellulose Characterization

Cellulose Nanofibrils (CNF) is an interesting nano-material with potential applications in composites, membrane technology, drug delivery, cell scaffolds, construction materials, packaging material and more. CNF have nanoscopic (_ 3□ _ 30 nm) diameters and lengths in the micrometer range. The project focuses on three-dimensional characterization of materials containing these fibrils with particular attention paid to porosity and interactions with other components.
The first goal of this project is to develop protocols for characterization of nanocellulose in hydrogels, films, membranes and paper using FIB/SEM and STEM as complementary techniques.
FIB/SEM (xy-resolution & 1:5 nm, z & 5 nm) can produce 3D images of samples
and prepare samples for STEM and TEM analysis. STEM offers higher resolution (xy & 0:4 nm) and may analyse smaller features of interest. Long term goals may include developing techniques to trace individual fibrils in the recorded images and map the network of pores present in these materials.
Techniques: FIB/SEM, STEM, image analysis
Relevant for: nanotechnologists, material scientists, biophysicists
Supervisor: Øyvind Weiby Gregersen, Professor, oyvind.w.gregersen@ntnu.no
Co-supervisors: Vegar Ottesen, Ph.D. candidate, vegar.ottesen@ntnu.no
Jonathan Torstensen, Ph.D. candidate, jonathan.torstensen@ntnu.no

Project proposal from Associate professor Størker Moe, *storker.moe@ntnu.no*

106 In this **Master with Purpose** project the assignment is to optimize Jatropha oil production and develop fast, easy and reliable methods to measure and control oil phosphorous, acid and water contents. The methods are to be employed in Kenya. The master will further include the use of advanced equipment at NTNU, in order to verify the functionality of the more simple developed methods.
The project is a collaboration between NTNU, Engineers Without Borders and ZERO - an organization working to minimize the human impact on climate. The given project can be either a project or master thesis, and is highly suitable for chemical engineers and chemists. We seek a person that is innovative and experimental by nature, and who enjoys analytical chemistry. This project is a gateway to a career in NGOs (Non – Governmental Organizations) or in analytical chemistry.
For more information about the project and information about the application, please use the QR- code below or visit the following link:
http://folk.ntnu.no/jonatht/biodrivsto_kenya.pdf. You are most welcome to send an e-mail (jonathan.o.torstensen@ntnu.no) and stop by for an informal meeting about the project.
Application deadline: 01. June 2015.
Supervisor: Størker Moe, Associate Professor storker.moe@ntnu.no
Co-supervisor: Lise Kvittingen, Professor lise.kvittingen@ntnu.no
Co-supervisor: Jonathan Torstensen, Ph. D. candidate jonathan.o.torstensen@ntnu.no

107 Use of mineral acid mixtures in concentrated acid hydrolysis of lignocellulose

The concentrated acid hydrolysis process has recently seen renewed interest after the development of acid recovery processes, due to its low processing temperature, high yields, low production of sugar degradation products and robustness towards raw material variation.

The most commonly used acid in concentrated acid hydrolysis for saccharification of lignocellulose is sulfuric acid. However, the use of sulfuric acid alone has a profound impact on the biomass, and combinations of sulfuric acid with other mineral acids like phosphoric acid are interesting modifications to the concentrated acid hydrolysis process.

The aim of the project will be to investigate the effect of different sulfuric acid/phosphoric acid mixtures on the saccharification process, by performing several hydrolysis experiments and quantifying sugar yields by HPLC. If the candidate is familiar with multivariate experimental planning, such methods should preferably be used in the design of the experimental matrix.

Supervisor: Størker Moe