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.

Project is reserved for Thomas S. Hemminghytt

Main supervisor: Prof. De Chen

Co-supervisors: Prof. Erling Rytter, Dr. Xuezhi Duan
Multifunctional proppants for kerogen conversion 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 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.

Project reserved for Isaac Yeboah.

Main supervisor: Prof. De Chen

Co-supervisors: Prof. Erling Rytter, Dr. Xuezhi Duan

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 CuCl₂ catalyst often used as oxychlorination catalysts. The present work focuses on the catalyst preparation and characterization of K, La and Mg modified CuCl₂ 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. A summer job at the Catalysis group is available.

Project reserved for Endre Fenes.

Main supervisor: Prof. De Chen

Co-supervisors: Martina Francisca Baidoo and Terje Fuglerud (INEOS)

One-pot conversion of biomass to chemicals on Ni/ZnO based 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 pyrolysis (bio-oil as intermediate), hydrolysis (sugars as intermediates) and gasification (synthesis gas as intermediates). 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.

*Project reserved for Siri Foss Morken.*

*Main supervisor: Prof. De Chen*

*Co-supervisor: Cornelis Gerardus van der Wijst*

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**Catalytic conversion of oxygenates to fuels**

This project deals with catalytic conversion of biomass derived oxygenates to fuels on multifunctional catalysts integrating the function of aldol condensation, ketonization 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.

*Project reserved for Astri Karin Torvik Jenssen.*

*Main supervisor: Prof. De Chen*

*Co-supervisor: Cornelis Gerardus van der Wijst*

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**Understanding of chain growth in F-T synthesis by kinetic study**

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

*Project reserved for Hanne Marie Straume.*

*Main supervisor: Prof. De Chen*

*Co-supervisors: Prof. Anders Holmen, Dr. Cristian Ledesma Rodriguez*

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**Autothermal dry reforming of methane**

Combined total combustion and dry reforming will be studied in a fixed bed reactor. Ni-Co catalysts with different Ni/Co ratio will be synthesized and tested in the reaction. The operating conditions, particular the ratio of O2/CO2/CH4 will be studied as a function of activity, CO/H2 ratio and carbon formation. The catalytic combustion of methane will be focused in the project.

*Main supervisor: Prof. De Chen*

*Co-supervisor: Prof. Anders Holmen*
Catalysts for electrochemical CO₂ reduction
Nanocarbon-Copper based materials are very interesting catalysts for electrochemical reduction of CO₂. Of the pure metals, Copper is the best catalyst for the electrochemical CO₂ 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.

Main supervisor: Prof. De Chen
Co-supervisor: Ida Hjorth

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.

Project reserved for Haakon M. V. Rui.

Main supervisor: Prof. De Chen
Co-supervisor: Dr. Wei He

Professor Magnus Rønning, magnus.ronning@ntnu.no

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 C₅⁺ 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 projects 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. One possible surface reaction is with trimethylsilyl chloride according to

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

thereby giving a silanized hydrophobic surface. Other surface modifiers will also be considered. The catalysts will be characterized using chemisorption and XRD. The reaction path of the anchoring on the surface will be followed by FTIR spectroscopy before the Fischer-Tropsch synthesis testing.

The project is reserved for Ata ul Rauf Salman

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

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

Doped nanocarbons represent a new class of metal-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 N-doped carbon nanofibres (N-CNF) show many properties that are markedly different from those of undoped counterparts. The N-CNF will be synthesised using supported or unsupported monodisperse Fe particles. The work will involve optimisation of the synthesis method in terms of particle size and support interaction. 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 method 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.

The project is reserved for Anne Barsnes

Supervisor/co-advisors: Professor Magnus Rønning/ Marthe Emelie Buan, Navaneethan Muthuswamy

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\textsubscript{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 10-20 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 N₂O.

The project is reserved for Øyvind Juvkam Eraker

Supervisor: Professor Magnus Rønning. Co-advisors: Sara Boullosa Eiras and David Waller, Yara Technology Centre

Fischer-Tropsch synthesis catalysts for CO₂-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 BTL plants. The catalysts need to be improved with respect to higher temperature, high CO₂ feeds, and improved durability.

The aim of this project is to develop catalysts that can operate at elevated temperatures (>250°C) with high carbon efficiency (C₅⁺ selectivity). The project will involve synthesis, characterisation and testing of Fe-based FT catalysts. The characterisation will involve chemisorption, XRD, TGA-DSC, TPR and S(T)EM.

The project is reserved for Lise Saue Jensen

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

Studies of methanol synthesis catalysts
The annual production of methanol at the Tjeldbergodden methanol synthesis plant at Nordmøre is about 900 000 tonnes. It is the largest methanol plant in Europe. Commercial methanol synthesis catalysts usually consist of CuO/ZnO/Al₂O₃. Two main deactivation processes take place on this catalyst system; thermal sintering and catalyst poisoning. This project will evaluate deactivated catalyst from the Tjeldbergodden methanol plant, mainly through catalyst testing in a Berty recirculation reactor.

The project is reserved for Stine Hagen Wigum

Supervisor: Magnus Rønning

Co-supervisor at Statoil: Øyvind Borg

Photocatalytic H₂-production through photo-reforming of hydrocarbons
Producing hydrogen from photoreforming of hydrocarbons is an emerging field within renewable energy research. Photocatalysts that can operate at ambient temperature without producing harmful by-products are ideal as environmentally sound catalysts. For such systems to be considered in large-scale applications, photocatalytic systems that are able to operate effectively and efficiently in a continuous flow reactor must be established. The project involves synthesis and characterisation of
new efficient nanomaterials with tuneable bandgap, and also testing of the catalyst materials in photocatalytic reactions such as photoreforming of methanol, ethanol and glycerol.

**Supervisor:** Magnus Rønning

**Co-advisor:** Charitha Udani
Colloid and Polymer Chemistry

Professor Johan Sjöblom, johan.sjoblom@ntnu.no

Study of droplet-droplet coalescence: effect of model demulsifiers on aged asphaltene-covered droplets

In the petroleum industry, demulsification is the process of breaking emulsions to separate the water from the rest of the crude oil. Chemical demulsification refers to the addition of certain chemicals, typically in the order of 1 up to 1000 ppm to promote phase separation. Essentially, the way demulsifiers act is by replacing and/or displacing the indigenous surfactants (i.e. Asphaltenes) adsorbed at the interface. The elastic film is therefore broken promoting coalescence.

In this project, the coalescence of asphaltene-stabilized droplets will be studied with the drop-drop micromanipulator apparatus, a device dedicated to the studies of the direct interaction between droplets or bubbles. The coalescence time, and the influence of a model demulsifier will be evaluated.

This project is a part of the Joint Industrial Program 1 project, a project sponsored by several central oil companies and chemical vendors. The work will be done at Ugelstad Laboratory, Department of Chemical Engineering.

Qualification requirements/prerequisites: Basic chemistry laboratory skills

Main supervisor: Professor Johan Sjöblom.
Co-supervisor: MSc. Diego Pradilla

De-Emulsification of Crude Oil Emulsions by Magnetic Surfactants

During oil production, water-in-oil emulsions are spontaneously formed when oil and water are mixed together. This process is controlled by the surface active natural surfactants, asphaltenes and resins, contained in the crude oils. These emulsions need to be destroyed after oil has been produced from the reservoirs in order to recover the oil. Several techniques exist to speed up the de-emulsification in particular the injection of cocktail of chemicals named de-emulsifiers in separator.

In 2012 Brown et al. have synthesized new surfactants which have the particularity to have their interfacial properties modified in presence of a magnetic field. These new magnetic surfactant could be a promising way to design a new family of de-emulsifiers for crude oil production. In this master thesis, magnetic surfactants will be prepared. Their interfacial properties with and without magnetic field will then be assessed before testing their de-emulsification efficiency on crude oil emulsions.

This project is a part of the Joint Industrial Program 1 “Mitigation and Remediation of Water-in-Crude Oil Emulsions with Complex Interfaces” project, a program sponsored by several central oil
Magnetic Nanoparticles for Extraction of Naphthenic Acids from Crude Oils
Production of acidic crude oil is in the near future expected to grow in importance. This acidity is mainly due to the presence of naphthenic acids (NA), which are a complex mixture of cyclic, acyclic and aromatic carboxylic acids. The presence of these molecules is associated with several problems occurring during crude oil production.

The goal of this master thesis is to develop new methods to extract NA from the crude oil by using magnetic functionalized nanoparticles. First the extraction and the recovery of model naphthenic acids in model solvents by commercially available magnetic functionalized nanoparticles will be studied. After optimizing extraction parameters and structure of the magnetic nanoparticles, the extraction will be tested on real crude oil systems.

This project is a part of the Vista Project “Functionalized Nanoparticles to Improve Crude Oil Quality”, a program sponsored by Statoil. The work will be done at Ugelstad Laboratory, Department of Chemical Engineering.

This subject is reserved for Mia Elise Ronander (miaer@stud.ntnu.no).

Supervisor: Johan Sjöblom
Co-supervisor: Dr. Galina Rodionova

Filtration of Emulsions
Description: Study of transport ability of emulsion droplets with different sizes through porous solid materials with different pore size. The study will involve droplet characterization before and after filtration through the pores. The characterization will be done with low field NMR and microscopy.

The work will be done at Ugelstad Laboratory, Department of Chemical Engineering.

This subject is reserved for Trine Nisja.

Supervisor: Johan Sjöblom
Co-supervisor: Laboratory Manager Camilla I. Dagsgård
Mechanism of Gel Formation between Tetra-Acid and Divalent Cations Determined by Calorimetry

Tetra-acid (also known as Arn) is a molecule present in petroleum crude oil at low concentration, typically the ppm level. This molecule can precipitate with calcium present in produced water to form deposits. These deposits have an impact on oil production and can even lead to costly shut-down. That is why it is important to determine the formation mechanism of these deposits.

The goal of this subject is to study the formation of gel in aqueous solution by reaction between tetra-acid and calcium. Different parameters will be measured such as the minimum bulk concentrations of tetra-acid required to react with Ca$^{2+}$, Ba$^{2+}$, Sr$^{2+}$, Mg$^{2+}$. The conditions for gel formation in bulk will also be determined. The main experimental technique will be isothermal titration calorimetry (ITC). This technique provides direct thermodynamic data about the reaction investigated. After data analysis, thermodynamic parameters such as reaction enthalpy, entropy and equilibrium constant can be determined.

This project is a part of the Joint Industrial Program 2 project “Mechanism of Formation of Calcium Naphthenate Gel: From Interfacial Reactions to Gel Formation”, a program sponsored by several central oil companies and chemical vendors. The work will be done at Ugelstad Laboratory, Department of Chemical Engineering.

Supervisor: Johan Sjöblom
Co-supervisor: Dr. Duo Wei

Reaction between Tetra-Acid and Calcium in Emulsion Followed by Zetametry

Tetra-acid (also known as Arn) is a molecule present in petroleum crude oil at low concentration, typically the ppm level. This molecule can precipitate with calcium present in produced water to form deposits. These deposits have an impact on oil production and can even lead to costly shut-down. That is why it is important to determine the formation mechanism of these deposits.

The goal of this subject is to study the reaction between tetra-acid and Ca$^{2+}$ at the interface between oil and water in an emulsion. This reaction will be followed by electrophoretic (zetapotentials) measurements to extract information on the degree of neutralization after reaction with Ca$^{2+}$, surface potentials and surface areas (when the droplet sizes are known). The influence of the presence of a calcium naphthenate inhibitor will also be studied.

This project is a part of the Joint Industrial Program 2 “Mechanism of Formation of Calcium Naphthenate Gel: From Interfacial Reactions to Gel Formation”, a project sponsored by several central oil companies and chemical vendors. The work will be done at Ugelstad Laboratory, Department of Chemical Engineering.

Supervisor: Johan Sjöblom
Co-supervisor: Dr. Duo Wei
Study the correlation between relative viscosity of crude oil emulsions and droplet size distribution.

Introduction
One challenge regarding emulsion viscosity of crude oil emulsions (w-i-o) is to understand and manage the change in emulsion viscosity, due to decrease in droplet size. It is a common understanding that a decrease in droplet size gives an increase in emulsion viscosity. At low water cuts the emulsion viscosity normally follows Pal and Rhodes (1985) or Rønningen (1995). At higher water cuts (prior to the inversion point) the relative viscosity of the emulsion is even more dependent on droplet sizes.

The assignment
Emulsion viscosity measurements of several different crude oils (with low and high viscosity), different water cuts and with use of varying shears, should be performed in a rheometer. Afterwards, the droplet size distribution of the emulsions should be measured. When the crude oil and water are emulsified and measured in-situ in rheometers, only small samples of emulsion is available. It is desirable to find a method for measuring the droplet size distribution on these small samples (10-20 ml) of emulsions. As a proposal, use of NMR and/or Mastersizer should be considered for droplet sizes measurements.

Prior to the experiments, a short literature study of existing reports and papers regarding emulsion viscosity and droplet sizes should be performed.

Additional
As an additional assignment, if there is more time and if necessary equipment is available, a comparison of relative viscosity and droplet sizes generated and measured in rheometer and flow loop should be performed.

Before the additional assignment is started, a literature study regarding the topic, should be carried out.

Laboratory facilities
The experiments should be performed at Ugelstad laboratory and/or at the laboratory at Statoil Research Center Trondheim.

Qualification
General understanding of crude oil rheology would be preferred

Supervisor: Johan Sjöblom

Co-supervisor: From Statoil, Anne Rossbach Hammer will facilitate the Master assignment

On the solubility of calcium in crude oils
Statoil has in the past executed a number of R&D activities related the formation and deposition of calcium naphthenates in oil production systems. A major breakthrough in this research was the ARN acid discovery. ARN is a 4-protic acid that tends to react with calcium ions in the formation water and create calcium naphthenate salt. Calcium naphthenate is neither soluble in the crude oil nor in
the produced water. Consequently the naphthenate creates a separate phase that over time accumulates in the crude/water interphase. The concentration of ARN in crude oils is normally very low, i.e. 0-100 ppm.

Another type of naphthenate is the so-called oil-soluble calcium naphthenate which is believed to be a salt formed by a reaction between the mono-parotic acids in the crude oil and calcium ions present in the formation water. The mono-parotic acids are very different from the ARN acid and the concentration of these acids can be as high as 1-10 weight% of the crude oil.

Statoil has developed several experimental methods for isolation and characterization of naphthenic acids in crude oils. These methods will be made available and the candidate will be guided in the use of them.

The present work addresses itself to the formation of oil-soluble calcium naphthenate according to the following reaction equation;

\[ 2 \text{RCOOH (oil)} + \text{Ca}^{2+} \text{(water)} = \text{Ca (RCOO)}_2 \text{(oil)} + 2\text{H}^+ \text{(water)} \]

The main objective for this master thesis is to collect experimental data and knowledge related to how the crude oil – and water compositional parameters influence this equilibrium... Of special interest is to characterize the structure of the naphthenic acids forming oil-soluble naphthenate.

The work will be performed at Statoil R&D, Rotvoll.

**Supervisor: Johan Sjöblom**

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**Demulsification by combining chemical demulsifiers and electrical fields.**

Oil continuous emulsions cause severe problems in the offshore processing offshore. A traditional way to solve the problem has been to add chemicals, so-called demulsifiers. However, recent development has also included electrostatic destabilization of the w/o emulsions. A leading company here is Wärtsilä Oil and Gas in Norway.

This student project will focus on a combination of the two strategies mentioned above. Fundamental questions to be answered will be how the electric field will change the fundamental properties of the demulsifiers (measured in HLB units). Destabilisation tests will be performed at Ugelstad Lab and Wärtsilä lab in Oslo.

**Supervisor: Johan Sjöblom**

**Co-supervisors: Sebastien Simon at Ugelstadlab and NN at Wärtsilä.**

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**Graphene oxides as emulsion stabilisers.**

Graphene oxides represent novel nanotechnology molecules that can be chemically modified both with a higher polarity (hydrophilic) and lower polarity (hydrophobic). These chemical modifications will determine the solubility of the molecule in oils and in water. The balance between the moieties
will render the molecule surface active properties. The task here will be a collaboration between the group for catalysis (Prof De Chen) and UL (Sjöblom/Simon).

Prof De Chens group will do necessary chemical reactions with the graphee oxide molecule in order to achieve surface active molecules, while UL will study how these molecules will stabilize emulsions, both water-in-oil and oil-in-water. Stability mechanisms will be mapped and the GO molecules will be compared with traditional surfactants. Interfacial properties will be documented with the advanced instrumentation available at UL. The project will be a collaboration between De Chen / Sjöblom and Simon.

**Supervisor:** Johan Sjöblom

**Co-supervisors:** De Chen and Sebastien Simon

**Associated professor Kristofer Gunnar Paso, kristofer.g.paso@ntnu.no**

### Next-generation wax inhibitors for the oil and gas industry

**Location:** Ugelstad Laboratory, Department of Chemical Engineering

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\(^1\) will be morphological modulation, effecting compact spheroids with reduced propensity to gel. A secondary mechanism\(^2\) 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, and quartz crystal microbalance. 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.

![Figure 1](image.png)

**Figure 1. Impact of morphological and chemical modulation on waxy fluid rheology**

**Supervisor:** Kristofer Gunnar Paso
Modeling Interfacial Mass Transport in Emulsions

Description:
The stability behavior of emulsions is a very important phenomenon in various chemical industries such as food, cosmetics, coatings, biotechnology, and petroleum. In this project, a model for interfacial mass transport and adsorption of model crude oil surfactants will be constructed, solved and analyzed. The goal is to understand how the basic emulsion properties, surfactant molecular properties, and water chemistry influence the interfacial composition and stability of emulsions. The modeling approach is general in order to be applicable to numerous chemical processes involving emulsions. The student should have basic skills and enthusiasm in computer programming and mathematics. Having completed the courses in colloid chemistry and transport phenomena is advantageous. In particular the student should be familiar with the concepts of adsorption and ionic chemistry along with the basic theory as well as constructing mathematical models (systems of differential equations) and the basic approaches for solving them.

Possible reserved candidates: Rakel Ekholdt, Ruth Elisabeth Sveen

Supervisor: Brian Grimes (brian.grimes@ntnu.no)

Co-supervisor: Aleksandar Mehandzhyiski

Molecular Simulation of Surfactants at Liquid-Liquid Interfaces

Description:
The chemical and thermodynamic properties of amphiphilic surfactant molecules at liquid-liquid interfaces influence the macroscopic behavior of a myriad of chemical systems from the home kitchen to oil platforms out at sea. In this project, molecular dynamics (MD) simulation amphiphilic molecules (surfactants) at liquid-liquid interfaces will be performed. The goal is to understand how the basic chemical structure of surfactants, the polarity of the oil phase, and ion composition of the water phase influences the geometric structure and energy of the interfacial surfactant layer. The student will learn the basics of MD simulation both theoretically (learning the physical mechanisms involved and how they are built into the methodology) and practically (learning the software to run MD simulations). The student should have basic skills and enthusiasm in computer programming and mathematics. Having completed the courses in colloid chemistry and transport phenomena is advantageous. In particular the student should be familiar with the concepts of adsorption and ionic chemistry.

Possible reserved candidates: Rakel Ekholdt, Ruth Elisabeth Sveen

Supervisor: Brian Grimes (brian.grimes@ntnu.no)

Co-supervisor: Aleksandar Mehandzhyiski
**Environmental engineering and reactor technology**

**Professor Hallvard Svendsen, hallvard.svendsen@ntnu.no**

**Calorimetric measurements with CO₂ capture solvents**
Heat of absorption and heat capacity of CO₂ capture solvents are very important parameters necessary for the design and operation of CO₂ capture plants. These data are necessary for example for the estimation of energy consumption for solvent regeneration. Accurate experimental data measured using calorimeters are therefore of high interest. The work will be done in collaboration with SINTEF and a conference or journal publication will/may be prepared based on the results from this project work.

Experimental work will include:

- **Measurement of the heat of absorption** of CO₂ with different solvents in the reaction calorimeter. The experimental procedure for this work has been developed earlier. The heat of absorption will be measured as a function of temperature, CO₂ loading and solvent composition.
- **Measurement of the heat capacity**. The experimental procedure recommended by the producer of the calorimeter will be tested and verified first. The heat capacity will be measured as a function of temperature and solvent composition.

**Main supervisor: Hallvard Svendsen**

**Co-supervisors: Inna Kim (SINTEF), Hanna Knuutila**

**Thermodynamics of CO₂ capture solvents**
Different companies and research groups around the world are working on the development of novel solvent systems in order to reduce capital and operational cost of CO₂ capture. The size of the absorber (capital cost) depends on how fast CO₂ reacts with a solvent (reaction rate). The reaction rate in its turn often depends on basisity of the amine, Kₐ. Data on Kₐ and its temperature dependence are often not available for the novel solvent systems and need to be measured. The work will be done in collaboration with SINTEF and a conference or journal publication will/may be prepared based on the results from this project work.

The project work will include:

- **Measurement of the pKa** for different solvent systems using potentiometric titration. The experimental procedure for this work has been developed earlier. pKa will be measured as a function of temperature and ionic strength of the solution.
- Calculation of the enthalpy of protonation based on the temperature dependence of the pKa.
Kinetics and physical solubility in CO₂-absorbent systems
The kinetics will be measured using string of discs (SDC) apparatus. Mass transfer rates will be measured for both CO₂ 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 models. Physical solubility of CO₂ into the solutions, density and viscosity are necessary data for the kinetic modelling and will be additionally measured. Solubility measurements are based on the so called N₂O analogy.

The work will be part of BIGCCS project and the plan is to prepare a conference publication based on the results.

Strong bicarbonate forming solvents
This work is part of EU-project Hipercap (http://www.sintef.no/Projectweb/HiPerCap/)

Bicarbonate forming systems are interesting partly because they may have a high capacity to bind CO₂ and, because it may be relatively easy to regenerate the CO₂ from the solvent. Based on this observation, it can be envisaged that bicarbonate formers with stronger basicity can lead to increased performance.

Work description: In this master thesis, equilibrium experiments will be performed to map the characteristics of various CO₂ – solvent systems regarding VLE for CO₂ and/or VLE in unloaded systems. The aim is to produce consistent sets of data for many solvent concentrations and for the temperatures 25, 40, 60, 80, 100, and 120°C. The data will be used to model the equilibrium behavior of the system. A conference or journal publication will/may be prepared based on the results from this work.
Simulation of pilot data with Aspen Plus
The objective of the master project is to simulate a CO₂ capture pilot plant located at NTNU using simulation tool Aspen Plus. The pilot is simulated with ASPEN plus using a rate based model. Thereafter the results are compared with existing experimental data from two separate pilot campaigns using 30wt% MEA as solvent. The difference between the campaigns is that different packing materials in the absorber and stripper were used. If time allows a third pilot campaign using another solvent will be simulated (the solvent will be decided later). The main objective of the work is to

- Build a validated simulation of the NTNU pilot plant in the Aspen.
- Compare the two different pilot campaign with 30wt% MEA and
- Gain knowledge of the limitations and flexibility of Aspen Plus.

Reserved: Trine Witzøe
Supervisor: Hanna Knuutila

VLE in precipitating carbonate systems
Carbonate systems has been suggested as promising solvents for CO₂ capture when combined with precipitation. However, there is lack of equilibrium data for CO₂-carbonate-water systems at relevant process conditions. These are needed to actually evaluate the real potential of such systems. The objective of this project is to measure vapor-liquid equilibrium data for potassium and sodium carbonate systems at temperatures and process conditions relevant for precipitating system. Based on the experimental data, the potential of these precipitating carbonate systems will be evaluated.

Main supervisor: Hanna Knuutila
Co-supervisor: Hallvard Svendsen

Professor Magne Hillestad, magne.hillestad@ntnu.no

Model predictive control of a polyolefin reactor
Cybernetica has, through many years, developed mathematical models of various polymerization processes. This includes processes for polyolefin production, phenol formaldehyde resins, PVC and emulsion polymerization. The models are deployed in production plants all around the world for online state estimation, model predictive control and online optimization.

Polyolefin processes of interest in this context are polypropylene and polyethylene based on Ziegler-Natta catalysts. The reactor types of interest include the slurry loop reactor, the liquid pool reactor and the fluidized bed reactor (gas phase). Polymers from propylene or ethylene are produced with
several different grades. A polymer grade is characterized by the melt flow rate (MFR), density and co-monomer content and other parameters. A polyolefin plant will produce several different grades and typically they will change grade 3-4 times a week. During normal operation and during grade transitions it is demonstrated that it is beneficial to apply nonlinear model predictive control.

The tasks for the work for the master candidate will be the following:

- Do a literature review of polyolefin reactor models applied for model predictive control.
- Develop a model of an industrial polyolefin reactor that is able to predict the dynamic response of the fluid concentrations and the polymer composition in addition to polymer properties such as melt flow rate (MFR).
- Implement the model in suitable programming languages.
- Verify the model against plant data and do offline model fitting.
- Develop on-line state and parameter estimation, i.e. select the measurements, states and parameters to be applied for estimation and estimator tuning.
- Develop a MPC control strategy of the reactor. Select the control variables (CV) and the manipulated variables (MV). Select the weights of CV and tune the penalty of MV move.

General purpose software for on-line model estimation, offline model fitting and nonlinear model predictive control, developed by Cybernetica, will be available for the candidate.

The topic is reserved for Kasper Linnestad

Supervisor: Magne Hillestad

Co-supervisor: Svein Olav Hauger from Cybernetica.

Professor Hugo Jakobsen, hugo.a.jakobsen@ntnu.no

Investigation of droplet breakage by single droplet experiments

The project contains a main part which consists in performing experiments in the laboratory using high-speed camera visualization of drop breakage in a stirred tank. The videos are then interpreted by use of the software KONK computing the breakage frequency (inverse breakage time), the number of daughters, the breakage probability and the daughter size distributions. The stirred tank is designed with a Rushton turbine and 4 baffles. The experiments should be repeated for 4-5 different distilled water-oil systems. If time allows, the experimental data should be used for population balance equation model validation. In particular, each of the underlying functions should be validated separately. Then, the population balance should be used and tested for the property of predicting known size distributions in dispersions.

Supervisor: Professor Hugo Jakobsen

Co-supervisor: Post doc Jannike Solsvik
**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.

**Supervisor:** Professor Hugo Jakobsen  
**Co-supervisor:** Post doc Jannike Solsvik

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**Population balance solution using the cell method**

Population balance equation (PBE) modeling is a very relevant task in multiphase reactor technology, phase separation in scrubbers, 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.

**Supervisor:** Professor Hugo Jakobsen  
**Co-supervisor:** Post doc Jannike Solsvik

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**Population balance breakage and coalescence closure discrimination**

Population balance equation (PBE) modeling is a very relevant task in multiphase reactor technology, phase separation in scrubbers, 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. 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. 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.

After all the existing breakage functions are considered, the more complex coalescence kernel functions should be evaluated in a similar manner. It might be convenient to postpone this task to the master thesis if time is limited at this stage.

Supervisor: Professor Hugo Jakobsen
Co-supervisor: Post doc Jannike Solsvik

Dynamic 2D bubble column model solution by collocation method
In this project a dynamic bubble column model should be solved by the collocation method being a method in the family of weighted residual methods. The two-fluid model equations for the flow in the reactor is the main task in this project, thus a cold flow study is the aim. This relatively simple model will be used to evaluate the advantage of the more complex combined multifluid-population balance models as have been developed earlier by previous PhD students in the group. The model can be implemented in the programming language MATLAB.

Supervisor: Professor Hugo Jakobsen
Co-supervisor: Post doc Jannike Solsvik

Modeling and simulation of a membrane reactor for hydrogen production from natural gas.
Several models for simulating hydrogen production from steam methane reforming combined with a hydrogen selective membrane for capturing CO₂ has been published in the literature. In this study the underlying model derivation should be verified and the correct model formulation should be solved and the results compared to model solutions provided in the literature. The model should be
derived based on the modeling principles given in the book “Chemical Reactor Modeling: Multiphase reactive flows”. The programming language will be MATLAB.

**Supervisor: Professor Hugo Jakobsen**

**Co-supervisor: Post doc Jannike Solsvik**

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

**Project 1: A HyMemCOPI Membrane Project**

The main objective of HyMemCOPI is to enable membrane technology to be efficient in combating GHG emission, by developing innovative hybrid (polymer + nanosized particles) membranes. A thorough study of the effect of the nanosized particles and their affinity and compatibility with the polymers will enable great improvements of the membrane fabrication and properties. CO₂ selectivity of more than 100, and permeance of more than $1 \text{m}^3(\text{STD})/\text{m}^2/\text{h}/\text{bar}^1$ through the hybrid membrane will be aimed, as we are eager to learn the scientific reasons behind the results and understand the transport phenomena through the membranes. HYMemCOPI’s objective of flux and selectivity lies on the “upper bound” of the Robeson line, and will enable membrane technology to become the next-generation CO₂ capture technology. The HyMemCopi-project is part of the BIGCCS-project coordinated by Sintef. The nanoparticles for the membrane will be provided by Sintef/Oslo and TNO in The Netherlands.

The main activities are:

- Manufacture of hollow fiber membranes, modifying nanoparticles and polymers.
- Study the transport mechanism of CO₂ in the hybrid material, and the effect of the functional nanosized particles varying variables such as pressure, humidity and mixture composition.
- Characterization of the membranes (DSC, TGA, SEM, FT-IR).
- Modify and further develop the hybrid material processing, in terms of both polymers and nanosized particles.
- Investigate the interaction of nanosized particles with the polymer matrix, ensuring improved compatibility and even distribution of nanosized fillers.

The results from HyMemCOPI will provide an understanding of the CO₂ transport mechanism through the membrane and how the nanosized particles affect the membrane properties. They will also take major steps toward a robust design and manufacturing of hybrid membranes.

HyMemCOPI will keep the advantages of the polymer membranes (flexibility, processability and low cost) and make a groundbreaking improvement in flux and permeability by integrating hybrid nanosized particles (down to less than 10 nm) in the polymer.
The candidate applying for the project should like to do experimental work, have knowledge about polymer chemistry, and preferably also membranes – this is however not so important.

**Supervisor:** May-Britt Hägg (hagg@nt.ntnu.no)

**Co-supervisor:** Gabriel Guerrero Heredia (Gabriel.g.heredia@ntnu.no)

### Project 2: Preparation of next generation mixed matrix membrane system for biogas purification

The separation of CO₂ from biogas is crucial in increasing the combustion value of generated biogas. Anaerobic digestion of biological resources and biological waste could be a promising technique to overcome waste problem along with alternative energy carrier. In a controlled reaction system, the gaseous mixture thus produced can contain up to 70% of biohydrogen and biomethane that can be used for commercial applications. Biogas, thus generated, contains significant amount of CO₂ which not only reduces its calorific value but their corrosive nature and reduces the possibilities to compress and transport over longer distances. Membrane technology is attractive for molecular scale separations because of its inherent advantages, such as low cost, high energy efficiency, ease of processing, excellent reliability and small footprint. Synthesis of membranes by introducing cross-linkable structures linked by using appropriate di-amines in the polymer backbone reduces the chances of plasticization, promotes chemical and thermal stability and improves membrane selectivity. Polymides containing a –C(CF₃)₂- link in the repeat unit eg. 6FDA have been found to increase both selectivity and permeability may be proposed for this study. Recently carbon nanotubes (CNTs) - functionalized single wall nanotubes (SWNTs) and metal organic framework (MOF) has found offer attractive gas transport properties may be proposed. In the project we will focus on the functionalized SWNTs

This project objective is on the development of mixed matrix membranes followed by characterization and membrane performance for relevant gas pairs (H₂/CO₂, CO₂/CH₄). The performance of membrane systems for the purification of biogas will be quite interesting in evaluating using appropriate modeling and simulation techniques in order to enhance energy contents efficiently.

The candidate should have some background on polymer chemistry and preferably also on membranes

**Supervisor:** May-Britt Hägg (hagg@nt.ntnu.no)

**Co-supervisor:** Sikander Rafiq (Sikander.rafiq@ntnu.no)

### Project 3: Pilot scale testing of fixed-site-carrier hollow fibers for CO₂ capture from flue gas

Globally, industry is responsible for one-third of all energy consumed and almost 40% of total world CO₂ emissions. A solution for reducing the greenhouse gas emissions to the atmosphere is carbon capture and storage (CCS). Chemical absorption processes are fully matured to achieve sufficient capture of CO₂, 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 CO₂ capture.

Membranes must overcome the trade-off between permeability and selectivity for CO₂ to compete with absorption. 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 project is financed by Gassnova and several other industrial partners: Statoil (Norway), Alberta Inovation (Canada), Air Products (USA). The research will be performed by NTNU, Sintef and Air Products.

The main objective of this project is to prepare pilot scale composite hollow fibers modules polyvinyl amine/ polysulfone with an area between 0.8 m² and 10 m² and to characterize them mainly by mixed gas (CO₂/N₂) permeation testing. The hollow fibers are based on polysulfone (PSf) polymer as porous support and selective layer of polyvinylamine (PVAm) for CO₂ from flue gas. Toward the end the produce membranes will be tested with real flue gas in Tiller CO₂ capture facility of SINTEF.

Scope of work of this project is as follows:

- Review the literature for fixed-site carrier membranes, coating techniques and gas separation properties of composite hollow fibers.
- The experimental work will consist of:
  1. Preparation by coating of the pilot scale hollow fibers module based on previous preparation parameters: polymer concentration, pH solution, drying time, temperature and packing density.
  2. Laboratory testing using various operational parameters: different gas flow rates, different configurations, different operational temperatures,
  3. Testing in real conditions with flue gas in Tiller.

The polysulfone hollow fibers modules to be coated will be received from Air Products (USA) through a collaborative project. The membranes will be investigated by scanning electron microscopy (SEM), gas permeation, and possibly other methods.

The candidate should have some background from polymer chemistry, and preferably also membranes, although not so crucial.

Supervisor: Prof. May-Britt Hägg (NTNU) (hagg@nt.ntnu.no)
Co-supervisor: Marius Sandru (SINTEF) (marius.sandru@sintef.no)

Project 4: Mass transport model design of Fixed-site-Carrier Polyvinylamine (FSC-PVAm) Membrane for CO₂ capture.

Global warming is becoming a world challenging issue related to the emission of greenhouse gases (GHG), especially CO₂. Three different options could be used for the reduction of CO₂ emissions, i.e.,
improve the energy efficiency of the processes, reduce fossil fuel consumption and CO₂ capture and storage (CCS). The key attraction of CCS is that we may continue to use fossil fuels without causing significant CO₂ emissions, which would be a most promising way to reduce the CO₂ emissions as required by the Kyoto protocol. Chemical absorption processes are fully matured to achieve sufficient capture of CO₂, 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 CO₂ 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 project is financed by Gassnova and several other industrial partners: Statoil (Norway), Alberta Inovation (Canada), Air Products (USA). The research will be performed by NTNU, Sintef and Air Products.

The goal of the project is to incorporate the chemical reaction in the current Chembrain code from the mass transport model, getting a suitable simulation tool for the facilitated transport through the membrane.

The candidate should have some background from mass transport, programing skills, and process simulation.

Supervisor: May-Britt Hägg (hagg@nt.ntnu.no)

Co-supervisor: Daniel Romero Nieto (daniel.r.nieto@ntnu.no)
Development of high flux composite membrane for membrane contactor used in pre-combustion CO₂ capture

Membrane contactors based on microporous hydrophobic materials already offer remarkable performances for different separation applications at industrial scale, especially for CO₂ capture. However, undesirable effects such as gradual changes in membrane surface morphology and/or partial wetting of the pores in membrane contactor can dramatically reduce the separation efficiency. A thin dense layer on a porous support, which has high gas permeability and high chemical stability, can be used to eliminate the pore-wetting. In this project different highly permeable polymers (Teflon 2400, PTMSP, PDMS) and porous support (PP, PVDF) are to be investigated to prepare an optimized composite hollow fiber membrane. The membrane CO₂ permeability and solvent (ionic liquids) compatibility will be tested in a long-term scale.

**Supervisor:** Assoc. Prof. Liyuan Deng  
**Co-supervisor:** PhD-student Zhongde Dai

Membrane contactor using ionic liquids for pre-combustion CO₂ capture

Membrane contactors are promising alternatives for CO₂ capture as they have larger interfacial area, better device-modularity and more operational flexibility compared with conventional absorption columns. This work focuses on CO₂ capture in gas–liquid membrane contactor using ILs as absorbents at pre-combustion conditions. Physical absorption ILs will be used as absorbent. Chemical absorption ILs (eg. Amino acid based ILs) blended with low molecular weight polymers (eg. PEG300) are an alternative absorbent. The influence of different operation parameters on separation performance in the membrane contactor will be systematically investigated including temperature, pressure, liquid/gas flow rate etc.

**Supervisor:** Assoc. Prof. Liyuan Deng  
**Co-supervisor:** PhD-student Zhongde Dai
Experimental and modeling study of CO$_2$ solubility in ionic liquids

Ionic liquids exhibit prominent thermo physical properties and are excellent solvent for CO$_2$ capture due to their low volatility, high thermal stability and high CO$_2$ absorption capacity. These aforementioned properties of ionic liquids make them prominent candidate for pre-combustion CO$_2$ capture process. Among these properties, CO$_2$ solubility in ionic liquids is important parameter.

The main tasks of this work include:

1. Experimental study of CO$_2$ solubility in ionic liquids at various temperatures/pressures
2. Parameter fitting of the experimental data

**Supervisor:** Assoc. Prof. Liyuan Deng  
**Co-supervisor:** PhD-Student Muhammad Usman

Adjunct professor Jana Poplsteinova Jakobsen, JanaPoplsteinova.Jakobsen@sintef.no

Pre-combustion CO$_2$ capture by absorption

Carbon Capture and Storage (CCS) is considered to be one of the most promising alternatives for reducing anthropogenic greenhouse gas (GHG) emissions, and is forecasted to account for 20% of the reductions in man-made GHG emissions in 2050. Pre-combustion CO$_2$ capture from coal sources is considered to be a promising option. Due to the high CO$_2$ partial pressure available, a solvent process based on Selexol is often considered due to low cost of this technology and its maturity. The parameters of this process has been set based on technical possibility (eg. 90% capture) however in practice an alternative set of parameters could be used in other to obtain a more cost efficient process.

The suggested master thesis work is therefore to simulate and design the pre-combustion Selexol CO$_2$ capture process from a coal power plant for different capture ratios using Aspen Plus. Based on these simulations, the sizes of the major process component will be evaluated in order to support a techno-economic analysis of the different process alternative.

**Skill requirements:**
Interest in environmental technology specifically carbon capture transport and storage (CCS).  
Interest in and some experience with simulations in AspenPlus.

**Supervisor:** Jana P. Jakobsen, jana.p.jakobsen@sintef.no  
**Co-supervisor:** Simon Roussanaly, simon.roussanaly@sintef.no
**CO₂ Capture – Thermodynamic expression for heat of absorption**

*Description of work:*
Gas absorption process using aqueous amine solutions is often considered to be one of the most promising technologies for capturing carbon dioxide (CO₂) from fossil fuel power plants. However, it is a very energy-intensive operation that will reduce the power plant output significantly. Heat of CO₂ absorption is an important factor for evaluating the heat balances and for energy assessment of the capture process. Heats of absorption of CO₂ with different solvents could be measured in a commercially available reaction calorimeter.

The objective of the work is to provide thermodynamic expression and possibly also a calculation procedure that could be used to predict heat of absorption. Such a procedure may be used for interpretation of experimental data from calorimetric measurements and to improve the thermodynamic models used in the absorber calculations.

The work will focus on formulation of thermodynamic expressions for the enthalpy of unloaded and loaded solution based on the theoretical thermodynamic paths from a standard state to the real system state. Expressions for the various additive contributions to the change of enthalpy along this path will be derived. Finally an expression for the heat of absorption will be proposed. In addition, the expressions available in the literature will be reviewed and discussed in light of the theoretical analysis. If time allows for that, a calculation procedure for heat of absorption based on the derived expression will be implemented in Matlab.

*Skill requirements:*
Interest in environmental technology specifically carbon capture transport and storage (CCS). Interest in and some experience with programming in Matlab.

**Supervisor:** Jana P. Jakobsen

**Co-supervisor:** Inna Kim, Hanna Knuutila

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**Safe transport of CO₂ – Thermodynamic properties of CO₂ rich mixtures**

*Description of work:*
Most of the international climate and energy organizations agree to day on the fact that CCS is a vital part of the least-cost portfolio of measures needed to address the climate change. In order to implement carbon capture, transport, and storage (CCS), safe and cost effective CO₂ transport infrastructure must be developed.

The objective of this work is to increase fundamental understanding of the behavior of CO₂ with impurities and potentially lead to improvements of the design and operation of CCS transport infrastructure with respect to safety, cost and efficiency. The work will focus on development of models and robust numerical algorithms for thermodynamic properties of CO₂ rich mixtures with the following impurities O₂, N₂, Ar, H₂, H₂O, CH₄, CO, SO₂. Different types of EOS will be investigated: cubic EOS, EOS based on the extended corresponding state principle (CSP) and EOS based on association theories. SINTEF ER’s in-house thermodynamic package already includes general formulation for cubic EOSs both 2 and 3 parameters with and without temperature and/or...
compositional dependant repulsion terms and in combination with either classic mixing rules like van der Waals and Excess Gibbs Energy Models like Huron-Vidal mixing rule SRK, PR, Patel-Teja, Schmidt and Wenzel. In addition, two CSP models are included for 1 and 2 fluid (SPUNG EOS and Lee-Kesler). The plan is to implement also representative models of the association theory based EOS such as CPA and PC-SAFT EOS and to combine Excess Gibbs Energy Models with the SPUNG EOS.

**Skill requirements:**
Interest in environmental technology specifically carbon capture transport and storage (CCS).
Interest in and some experience with FORTRAN programming.

**Supervisor: Jana P. Jakobsen, jana.p.jakobsen@sintef.no**

**Co-supervisor: Geir Skaugen, geir.skaugen@sintef.no**
Process-system engineering

Professor Sigurd Skogestad, skoge@ntnu.no

Autonomous PID control
The goal is to make a controller which retunes itself and which also adjust its own setpoint in order to optimize operation. This has been a goal in process control for 50 years, but one has not been able to make it work in practice. PhD candidate Vinicius de Oliveira has done some preliminary experiments which look very promising and we want to extend this work towards

PID control. The project will be a mix of experimental and theoretical.

Supervisor: Sigurd Skogestad

Optimal PID settings for first and second-order processes
The objective it test the improved SIMC PID tunings which were proposed by Grimholt and Skogestad (at DYCOPS in 2013) and compare with the optimal settings. The definition of "optimality" is important and in addition to performance (IAE) one needs to consider also robustness (Ms, time delay margin, gain margin, etc.) and input usage. The work is mainly theoretical, but one may also do some simple experiments.

Supervisor: Sigurd Skogestad

Optimal operation of ammonia plants
This is project in cooperation with Yara who operate mainly ammonia plants. It will mainly involve simulations using Hysys.

Supervisor: Sigurd Skogestad
Co-advisor: Julian Straus.

Associate professor Johannes Jäschke, johannes.jaschke@ntnu.no

Modelling and optimization of compact subsea separators
In order to be able to produce hydrocarbons economically from reservoirs under difficult circumstances, such as ultra-deepwater conditions or low reservoir pressure, is 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.

However, 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 can be challenging when controlling the process.

The objective of this thesis is to model and optimize a compact subsea separation process for control purposes. We will start from the model described in Ellingsen (2007), which can be found at [http://www.nt.ntnu.no/users/skoge/diplom/prosjekt07/ellingsen/](http://www.nt.ntnu.no/users/skoge/diplom/prosjekt07/ellingsen/), see also the figure below:

In this process liquid and gas coming from a well are to be separated, and the separation is done in two stages, where first the bulk separation is done in the Gravity separator, and then the gas-rich phase is sent to the deliquifier, and the liquid-rich phase is sent to the degasser. The operational objective is adjust the available valves in such a way that the gas content in the liquid stream to the pump is minimized.

We are looking for someone who likes to program in matlab or a similar language, with good mathematical skills the ability to work independently. The main focus of the project is on the modeling and steady state simulation of the process. In a possible follow-up master project, the focus will be on using the model for finding optimal operation strategies. The simulations will be done in the modeling languages matlab or ampl.

Reserved for Preben Fürst Tyvold, and Fahad Matovu,

**Supervisor: Johannes Jäschke**

**Co-supervisor: Sigurd Skogestad**

**Modelling and optimization of a 2-stage compressor train.**

This project has been suggested to us by Exxon Mobil, and it is similar to a process they want to optimize in one of their plants. The goal of this project is to model and optimize a 2-stage compressor cooling system with propylene as cooling fluid, see figure below (A very detailed process description...
A process stream is cooled down by a two-stage refrigeration system, where most of the cooling is performed at the low pressure (LP) evaporation stage, and the remaining heat is removed from the process stream in the intermediate pressure (IP) evaporator. The amount of cooling at the high and the intermediate pressure level can be adjusted by manipulating the control valves (XV1,XV2,XV3).

The objective of this project is to find an operation strategy, which adjusts the control valves such that the total shaft work W is minimized. This correspond to minimizing the total energy consumption.

We are looking for someone who likes to programm in matlab or a similar language, with good mathematical skills the ability to work independently. The main focus of the project is on the modeling and steady state simulation of the process. In a possible follow-up master project, the focus will be on using the model for finding optimal operation strategies. The simulations will be done in the modeling languages matlab or ampl.

Reserved for Adriaen Verheyleweghen

Supervisor: Johannes Jäschke

Co-supervisor: Sigurd Skogestad

Adjunct professor Krister Forsman, Krister.Forsman@perstorp.com

Optimization of multiproduct batch distillation

At site Perstorp there is a multipurpose plant, producing several different highly specialized products, batchwise. The synthesis step (batch reaction) is always followed by a batch distillation step. In the distillation, typically 4-5 different fractions are separated. The lightest component comes first, etc. Each fraction has a specified reflux flow. Whether to switch from the current fraction and start a new, heavier one, is determined by an online density measurement. Density is supposed to be proportional to concentration. This project consists in determining both optimal switching points for
the different fractions, i.e. densities, and optimum reflux flow for each fraction. The optimization criterion is to maximize production capacity, given that constraints on product purity and other quality parameters are met. The input to the analysis is historical data, collected in our process history database.

The limits currently used have been derived empirically over a long time, based on experience, and it is highly probable that they can be improved. This plant is capacity limited, meaning that extra tons produced can always be sold to the market. Thus large profit increases can be expected if the batch distillation process is thoroughly optimized.

**Supervisor: Krister Forsman**

**Co-supervisor: Sigurd Skogestad**

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**Professor Heinz.Prisig, 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.

**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**

**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**
Felles-lab, 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

Felles-lab, 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 understand their behaviour and check and if necessary improve the design of the injector and the sensor.

Supervisor and daily contact: Heinz A Preisig

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.

Supervisor : Heinz A Preisig, PhD student to be named.

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.

Supervisor Heinz A Preisig, PhD Student to be named.
Green chemistry, SINTEF cooperation: SINTEF Bio-Refinery Pretreatment of marine biomass

Partner is SINTEF materials and chemistry that has financed projects in this domain. Currently it is "Biomass and economy: Biobased products from sustainable resources". Cost-effective conversion of bio-mass is the main objective. The biomass is macro algae and target chemicals are intermediates, base chemicals and biofuel.

The biomass is microbiological converted. Objective is to generate a new preprocessing procedure and a enzymatic hydrolysis method with a minimum yield of 85%. The project involves both practical work in the lab working with enzymes steering the viscosity of the reaction mixture as well ad its hydrolysis. A following theoretical analysis should lead to a process design. The task will be adjusted to the student’s background.

Main supervisor: Heinz A Preisig

Co-supervisors: Inga Marie Aasen & Bernd Wittgents from SINTEF

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

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**

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**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**

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**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.

**Supervisor and daily contact: Heinz A Preisig**

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**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**

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**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.

**Supervisor and daily contact: Heinz A Preisig**

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**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
Cellulose III Nanofibrils and Films
Development of Production and Characterization Methods for a Novel Nanomaterial

Cellulose, the most abundant polymer on earth [1], is a biodegradable and renewable material which on the nanoscale has many interesting properties such as tensile modulus on-par with the best synthetic polymers such as Kevlar [2] or excellent oxygen barrier properties [3] making it an excellent candidate for many novel applications or as a sustainable alternative to current hydrocarbon-based solutions.

Cellulose comes in several crystalline forms, among them Cellulose I is found in nature whereas II, III and IV with subtypes are the result of modification of Cellulose I. Cellulose III is a less dense, more reactive form of cellulose which may be produced by submersion of cellulose I in liquid ammonia [4]–[6]. While nanocellulose derived from cellulose I is a topic for much study [7]–[10], Cellulose III based nanocellulose is to our knowledge only subjected to cursory studies [11], [12].

We propose a project focused on the properties of cellulose III based nanocellulose. Our proposed project consists of conversion of Cellulose I to Cellulose III and subsequent conversion of this to nanocellulose by high-pressure homogenization and the creation and characterization of films produced from this material.

Methods of interest include but are not limited to Electron Microscopy (SEM), X-Ray Diffraction (XRD) gas permeability tests and tests of optical properties as well as tensile modulus and elastic modulus.

This project will be a part of the research in the NANO 2021 project NORCEL coordinated by PFI.

Supervisor: Prof. Øyvind Gregersen
Co-supervisors: PhD-student Vegar Ottesen and Prof. II Kristin Syverud

Bibliography


