TKP4580/TKP4581 SPECIALIZATION PROJECT FALL 2017

DEPARTMENT OF CHEMICAL ENGINEERING

CATALYSIS

PROJECT FROM PROFESSOR EDD A. BLEKKAN EDD.A.BLEKKAN@NTNU.NO

1. THE EFFECT OF ALKALI ON COBALT-BASED FISCHER-TROPSCH CATALYSTS

Biofuels will play an important role in a future, sustainable energy system. We are studying several routes to converting lignocellulosic biomass to fuels, in this project we will investige aspects of the Fischer-Tropsch (FT) based Biomass To Liquids (BTL) processes. Ash components like alkali and alkaline earth species have been shown to deactivate cobalt-based FT catalysts [1-3]. Syngas cleaning and conditioning is therefore important, but costly steps in the process. It is important to understand how these compounds influence the catalysts, and the levels that can be tolerated. This is important information in the design of new processes. In this project we will work on aspects of the interaction between alkali compounds and supported cobalt catalysts. Such aspects could be the role of the counterion (e.g. chloride, hydroxide, sulfate or nitrates), and the role of the catalyst support (type of support (chemistry), or surface area. The work will be both theoretical (literature review) as well as experimental (catalyst preparation, characterization and testing).

Supervisor: Prof. Edd A. Blekkan. Co-supervisor: PhD-student Ljubisa Gavrilovic

PROJECTS FROM PROFESSOR DE CHEN DE.CHEN@NTNU.NO

2. SYNTHESIS OF SOLID SORBENTS AND KINETIC STUDY FOR CO_2 CAPTURE

Fossil fuel-fired power plants are the main contributors to the world energy resources at the moment and it is increasing in future (IEA 2008). It is expected that energy consumption will increase up to 45% until 20302. Since this demand will mainly be satisfied by producing power from fossil fuels, the emissions of greenhouse gases will continue to increase, unless carbon capture and storage (CCS) is coupled to power plants. Using a CCS technique, secure energy supply can be ensured from fossil fuels reducing the emission of CO2 to atmosphere and mitigating the global warming effect. Among the different CCS technologies, post combustion carbon capture process is the only option for the retrofitting of existing power plants. The present work deals with synthesis characterization of solid CO2 sorbents and pelletization to make spherical solid sorbents for use in a special reactor. The sorbents will be screened in terms of kinetics, capacities and stability in CO_2 capture. The kinetic study of carbonation and decarbonation reactions will be performed on the resulting solid sorbents. The project is performed with a close cooperation with the Fjell Technology Group, Gasnova, and SINTEF materials and Chemistry. At least two students can work in this project, one focuses on synthesis and screening and another focuses on the kinetic study.

Supervisors Prof. Edd A. Blekkan , Dr. Kumar R. Rout (SINTEF), Dr. He Li, Prof. De Chen

3. SYNTHESIS OF LOW TEMPERATURE SORBENTS FOR CO_2 CAPTURE

CO2 capture and storage (CCS) has attracted significant attention in the past decade due to the global warming issue. The current developed and developing CCS technologies are mostly targeted at capturing CO2 from large point sources, such as coal-fired power plants. In addition, solid sorbents are often required for removal of CO2 and H2S from natural gas, and synthesis gas from biomass and coal gasification. The present work deals with a development of carbon spheres with polyethylenimine (PEI). The polymer spheres will be synthesizedby ultrasonication assisted polymerization. The pore size will be controlled by addition of solid porogens (pore making agents) such as nanoparticles as templates. The CO2 uptake capacity and the stability will be studied as function of the molecular weight and loading of PEI.

Supervisors: Prof. Edd A. Blekkan , Dr. Kumar R. Rout (SINTEF), Prof. De Chen

4. KINETIC STUDY AND REACTOR MODELING OF ETHYLENE OXYCHLORINATION

The project deals with a reactor model for oxychlorination of ethylene in fixed bed multi-tubular reactors. Oxychlorination of ethylene is one of the steps in a balanced process for production of vinyl chloride (VCM), the monomer for production of polyvinyl chloride (PVC), one of the world's most widely produced thermoplastic.

Chlorination of ethylene $C_2H_4 + Cl_2 \Rightarrow C_2H_4Cl_2$ (EDC)

Thermal cracking of EDC $C_2H_4Cl2 \Rightarrow HCl + VCM$

Oxychlorination of ethylene $C_2H_4 + 2\ HCl + \frac{1}{2}\ O_2 \Rightarrow C_2H_4Cl_2$

Several types of reactor concepts can be used for the oxychlorination process. The reactor concept of interest for this modeling work consists of three multi-tubular reactors in series in a heat-exchanger (shell and tube) configuration. Ethylene and HCl are fed to the first reactor while the oxygen is fed as air and distributed between the reactors. The heat of reaction is removed by raising steam on the shell side of the reactors. The reaction temperature is controlled by the steam pressure. The aim of the project is to develop a two dimensional non-isothermal model that predict the impact of reactor parameters on temperature profiles and by-product formation. Rate expressions for the reactions, equations for heat and mass transfer and pressure drop parameters will be provided. Data from an industrial plant will be provided for evaluation of the model. At least two students can workon this project, one focusing on the experimental kinetic study on CuCl2 catalysts with different promoters, while another focuses on the kinetics and reactor modeling.

Supervisors: Dr. Kumar Ranjan Rout (SINTEF), and Terje Fuglerud (INEOS), Prof. De Chen

5. CATALYTIC CONVERSION OF BIOMASS DERIVED OXYGENATES TO FUELS AND CHEMICALS (H2BIOOIL)

H2BioOil is a promising process to convert biomass to fuels through fast pyrolysis, catalytic upgrading of pyrolysis vapor and hydrogen production by sorption enhanced reforming of byproducts in the process. This project deals with catalytic conversion of biomass derived oxygenates from pyrolysis to fuels and chemicals on multifunctional catalysts integrating the function of aldol condensation, esterification and hydrogenation. The project will deal with synthesis, characterization, and testing of bifunctional catalysts supported on carbon materials. The products will be thoroughly analyzed by GC-MS, HPLC, and work will be performed in NorBioLab. The candidates will work in the biomass conversion team.

Supervisors: Assoc. Prof. Jia Yang, Dr. Kumar R. Rout, Isaac Yeboah

6. *One-pot conversion of biomass to chemicals and fuels*

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 the intermediate). 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 algae. The work will be performed in NorBioLab.

Supervisors: Assoc. Prof. Jia. Yang, Haakon Rui, Prof. De Chen,

7. *Catalytic combustion of natural gas*

The catalytic combustion of methane is a key technology for the production of clean energy and for after-exhaust treatment. Its application in gas turbines (high temperature catalytic combustion – HTCC) leads to ultra-low emissions of CO, NOx and unburned hydrocarbons. Transition metal catalysts will be synthesized, characterized and tested for methane total combustion. The operating conditions will be optimized in terms of different applications. Kinetics of methane combustion will be also studied.

Supervisors: Assoc. Prof. Jia Yang, Shirley Elisabeth Liland, De Chen

Projects from Professor Hilde Venvik hilde.venvik@ntnu.no

8. *Oxidation of methanol to formaldehyde over Ag catalysts*

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.

Recently, all necessary equipment has been designed, installed and tested to enable detailed investigations of this reaction. Important issues include the effect of reaction conditions tuning on the selectivity, structural changes induced by the reaction conditions, interplay between heterogeneous and gas phase chemistry, and in particular the role of O and surface/bulk O species. 1-3 projects are offered, depending on the availability of instrumentation and interest of the candidates, centred on the following core activities:

1. Partial oxidation of methanol in an annular Ag reactor with possibility of including reactor modelling
2. Partial oxidation of methanol over granular Ag catalyst – kinetic investigations

3. Characterization of Ag catalysts and model systems by surface science techniques such as photoelectron spectroscopy (XPS/PES) and scanning tunnelling microscopy (STM)

The projects are 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.

Supervisors: Prof. Hilde Venvik, Associate Professor Jia Yang (SINTEF), Senior Scientist Rune Lødeng (SINTEF), postdoctoral fellow Mari-Helene Farstad. K.A. Rasmussen and Dynea personnel will also be engaged in the project.

9. *CATALYTIC METHANE ABATEMENT FOR NATURAL GAS ENGINES*

More and more stringent regulations on greenhouse gas and NOx emissions motivate the search into more environmental benign fuels than gasoline and diesel. Natural gas as an alternative fuel has the advantages of significantly reduced CO2 and NOx emissions, low S, and no particulate matters compared to conventional fuels. Natural gas is also worldwide available and can be applied efficiently in cars, buses, heavy-duty trucks, as well as marine vehicles. Marine machinery running on LNG is particularly relevant in a Norwegian context, with a strong position within the LNG value chain as well as in shipping, representing also an opportunity for reduced greenhouse gas and NOx emissions in the transportations sector. However, a critical issue of unconverted CH_4, typically termed methane slip, emerges due to the NOx suppression requirement on the engines. This has to be solved before wide application of CH_4 due to its extremely high greenhouse gas potential.

Exhaust after-treatment by catalytic combustion is a method with potential for achieving this, but state-of-the-art technology for methane abatement has still not reached a commercial maturity level. The challenge for CH_4 conversion is its high stability (no C-C bonds) compared to the higher hydrocarbons. Typical conditions that must be satisfied for efficient CH_4 removal are:

- CH_4 activation and conversion at low operating temperatures (< 500 °C)
- Fast light-off
- Efficiency at low CH_4 concentrations (< 1000 ppm),
- Tolerance to water vapour (10–15%), CO_2 (15%), and large excess of O_2
- Tolerance to low levels of SO_x (ca. 1 ppm, ~0 for LNG)

Combustion catalysts are typically based on noble metals or transition metal oxides. Platinum and palladium (Pt, Pd) are the most investigated noble metals, due to their generally favourable low temperature activity. However, their use are limited by the thermal stability, scarcity and high cost. Nickel and cobalt (Ni, Co) are among the most addressed transition metals with promising low temperature activity. The project targets development of Co, Ni based catalysts for low temperature methane oxidation at methane slip relevant conditions. The effect of catalyst promoter (Pd, Pt, CeO_2) will be investigated. The main research activity includes: Catalyst preparation, characterization, and catalyst testing in fixed-bed reactor.

This project will be part of an on-going project granted from the Research Council of Norway Transport 2025 program, entitled "EmX 2025 – an R&D base for reduced exhaust emissions in the Norwegian marine transportation sector". Industry enterprises involved in the project advisory board are Rolls Royce, Gassnor, Yara, as well as cooperation with Marintek (Now SINTEF Ocean)

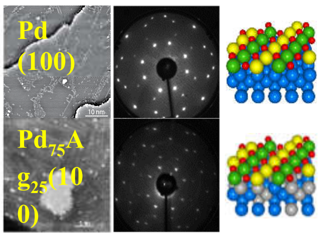
Supervisor: Professor Hilde Venvik, Associate Professor Jia Yang, Senior research scientist Rune Lødeng.

10 NANOSCALE INVESTIGATIONS AND MODIFICATIONS OF CATALYSTS AND CATALYTIC MODEL SYSTEMS

iCSI – industrial Catalysis Science and Innovation – is a Centre for research based innovation appointed by the Research Council of Norway and hosted by Department of Chemical Engineering, NTNU. Development of state-of-the-art research methodology is at the core of iCSIs generic activities, and includes investigating well defined catalyst model systems at the nanoscale. For this, scanning tunnelling microscopy (STM), X-ray photoelectron spectroscopy and low energy electron diffraction (LEED) are used in conjunction with first principles modelling by density functional theory (DFT). More recently, high resolution and so-called near-ambient photoelectron spectroscopy (HRPES and APPES) using synchrotron light has enabled increased precision and investigations under reaction relevant conditions. Recent results obtained at NTNU includes the understanding as K as a Co Fischer-Tropsch catalyst inhibitor and the effect of alloying elements to Pd on its catalytic properties (see figure below).

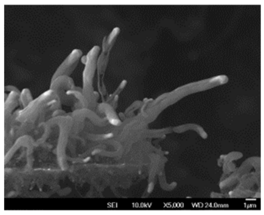
The project concerns experimental investigations on the atomic scale of metallic model systems relevant to the selective oxidation of methanol to formaldehyde over Ag, the hydrogenation of CO to long chain hydrocarbons over Co, and/or the effect of alloying elements (Ag, Cu, Au) on the properties of Pd towards oxidation and hydrogen permeation. The project is well suited for 1-2 students with an interest in experimental investigations of nanomaterials applied in the chemical industry or in emissions abatement. The laboratories are available at the Dept. of Chemical Engineering (IKP) as well as NTNU Nanolab, with the possibility of participating at synchrotron beam time if timing allows.

Supervisor: Prof. Hilde J. Venvik and Co-advisors: Post doc., Dr. Mari Helene Farstad (IKP), Research Scientist Dr. Ingeborg-Helene Svenum, SINTEF Materials and Chemistry



The figures show STM (left), LEED (center) images and atomic models of the (√5x√5)R27° oxide formed on Pd(100). A similar surface oxide structure is also obtained for $Pd_{75}Ag_{25}$(100). The (√5x√5)R27° palladium oxide is a highly active phase for CO oxidation on Pd, whereas chemisorbed oxygen has the same role on PdAg. Hence, the addition of Ag modifies the reaction mechanisms.

11 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 exposure to high carbon activity gas atmosphere at high temperature, 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 will may focus on alloys applied in so-called microstructured reactors (Inconel 800 series) for process intensification, exposures and advanced characterization of these, including use of Raman spectroscopy, as well as Auger electron spectroscopy with depth profiling by Ar ion sputtering, X-ray photoelectron spectroscopy and use of FIB/STEM at NTNU NANOLAB. Model systems for assessing specific, detailed phenomena may also be identified and investigated. The figure shows large C-filments growing on Incoloy 600 as imaged by SEM.

Supervisor: Prof. Hilde Venvik

Co-advisors: PhD student Xiaoyang Guo. Dr Estelle Vanhaecke (NTNU). Possible collaboration also with Karlsruhe Institute of Technology (KIT).

PROJECTS FROM PROFESSOR MAGNUS RØNNING MAGNUS.RONNING@NTNU.NO

12 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 catalyst 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 (<850Cº), 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 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: Professor Magnus Rønning, Co-advisors: Ole Håvik Bjørkedal, Rune Lødeng (SINTEF)

13 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 cost-efficient catalysts for achieving NO/NO_2 equilibrium for these applications. The work involves synthesis, characterization and activity measurements of suitable catalyst materials, and will be carried out in close collaboration with 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, INOVYN and Haldor Topsøe AS as industrial partners.

Supervisor: Professor Magnus Rønning. Co-advisors: Ata ul Rauf Salman, Bjørn Christian Enger (SINTEF), Rune Lødeng (SINTEF), Mohan Menon (Yara Technology Centre)

14 In situ characterization of industrial catalysts

Advanced characterization methods will be employed to study industrial catalysts in their actual working environment (in situ). The project deals with characterization of selected catalysts at industrially relevant conditions in terms of pressure, temperature and feed composition. The Catalysis Group is using an increasing number of advanced in situ techniques for catalyst characterization. Fourier Transform infrared spectroscopy (FT-IR) and Raman spectroscopy will be the primary techniques for studying catalyst performance in the first hours of operation. The in situ characterization techniques are able to provide information about phenomena such as catalyst structure, deactivation, reaction intermediates and surface acidity.

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, INOVYN and Haldor Topsøe AS as industrial partners.

Supervisor: Professor Magnus Rønning. Co-advisor: Samuel Regli

Projects from Associate Professor Jia Yang jia.yang@ntnu.no

15 Biopolymers Assisted Preparation of Iron based Fischer-Tropsch Catalysts

This project utilized nature biopolymer as a soft template for preparation of highly dispersed iron catalysts for Fischer-Tropsch synthesis. The synthesis method involve a sol-gel method followed by combustion. The effect of biopolymer type and synthesis conditions will be explored. The structure and performance relationship will be established through several characterization techniques. XRD, BET, Chemisorption, SEM, TEM, TGA will be used to characterize the structural, morphology of the metal oxides. The synthesized material will be tested in a fixed bed reactor for Fischer-Tropsch reaction, which is an important step in transformation of Biomass to biofuels. This project will be part of ongoing PhD project.

Supervisor: Associate professor Jia Yang (Jia.Yang@ntnu.no)

Co-supervisor: Professor Anders Holmen

16 Polymer Assisted Synthesis of 2D and 3D Carbon Supported Materials for Catalytic application

The project explore the potential of using nature polymer for synthesis of 2D and 3D materials for catalytic application. Main task involve material synthesis with special focus on the optimization of synthesis methods on the morphology and properties of the materials. Characterization with SEM, TEM, TGA, XRD, BET, Chemisorption will be used as a feedback to direct further synthesis. Possible applications in oxygen reduction reaction (ORR) or photo catalysis will be tested. The main research activities will be carried out at the Catalysis Group in the Department of Chemical Engineering.

Supervisor: Associate professor Jia Yang (Jia.Yang@ntnu.no)

Co-supervisor: Professor Bjørn Erik Christensen (Department of Biotechnology)

17 Artificial Photosynthesis-Visible Light Photocatalysis for Water Splitting

Solar energy is the most abundant energy source available on earth. Nature utilize solar energy through green plant via photosynthesis to produce chemical energy. Artificial photosynthesis provide an attractive though challenge rout to produce energy carriers, such as H_2 and chemicals. Currently, the main challenge is the low energy efficiency. This project focus on the develop TiO_2 or ZnO based photocatalyst for visible light water splitting. The project involves literature review, catalyst synthesis, characterization and testing.

The effect geometry, structure and dopants will be explored using diverse characterization techniques, including SEM, TEM, TGA, XRD, BET, Chemisorption. The catalysts will be tested for visible light water splitting in a semi-continuous reactor.

Supervisor: Associate professor Jia Yang (Jia.Yang@ntnu.no)

Co-supervisor: Professor Magnus Rønning

Surface and Colloid chemistry

Projects offered by Professor Johan Sjöblom johan.sjoblom@ntnu.no

18 Characterization of naphthenic acids from crude oil

Naphthenic acids are a group of cycloaliphatic, acid functional compounds naturally occurring in crude oils. Because of their acidity naphthenic acids cause problems in different part of the oil production such as corrosion of pipes and vessels and chemical degradation of polymeric materials, like polyamides.

Polyamide 11 (PA11) is a common material used in flexible risers. Polyamides undergo degradation by hydrolysis. The rate of reaction increases with temperature and in the presence of acids. Flexible risers are complex structures which are demanding and expensive to replace. A method for predicting the remaining life time of a flexible riser in operation based on exposure scenario and oil quality would therefore be highly beneficial to the oil industry.

Naphthenic acids are known to play a role in the degradation of PA11 in flexible risers. In this project

- naphthenic acids from one oil field will be isolated and characterized
- A degradation study will be performed, where PA11 is exposed to naphthenic acids in a controlled environment and the impact on material properties is monitored.
- Exposure of PA11 to a medium containing dissolved, isolated acids. The composition of the medium is analyzed as function of time to monitor any changes in acid composition.

The project is a cooperation with Statoil.

Supervisors (NTNU): Are Bertheussen, Johan Sjöblom (professor), Ugelstad Laboratory, IKP, NTNU

Contact persons, Statoil: Ingvild Johanne Haug, Heléne Vrålstad (HVRA@statoil.com)

19 Improvement of Efficiency of Green Demulsifiers by Interplay with Electrocoalescer

During petroleum crude oil production there is incorporation of water in oil under the form of emulsions i.e. droplets of water in the oil phase. These emulsions need to be "broken" to obtain anhydrous oil and pure water. This is industrially done by different methods like heating, adding chemicals named demulsifiers, applying an electrical field (electrocoalescence) and so on. As environmental regulations become more rigorous, it is of outmost importance to improve oil-water separation technology in order to successfully process increasingly complex production fluids

This work will focus on the determination of the synergy and interplay between green chemical demulsifiers and electrical fields in the destabilization of crude oil emulsions. The destabilisation efficiency of green demulsifiers will be determined without and with electrical field using a new electrocoalescer developed in-house. Nuclear magnetic resonance (NMR) will be used to determine the efficiency of separation by measuring the droplet size distribution of emulsions as well the oil-water separation rate.

This project is a part of the *Joint Industrial Program "New Strategy for Separation of Complex Water-in-Crude Oil Emulsions: From Bench to Large Scale Separation"*, a project sponsored by the Norwegian Research Council and several central oil companies and chemical vendors. The work will be performed at Ugelstad Laboratory, Department of Chemical Engineering.

Supervisor: Prof. Johan Sjöblom.

Co-supervisors: Dr. Sameer Mhatre and Sébastien Simon.

20 UNDERSTANDING THE INTERACTIONS BETWEEN NAPHTHENIC ACIDS AND ASPHALTENES TO IMPROVE SUBSEA SEPARATION

Part of the complete subsea factory envisioned by several oil companies is to produce export quality crude oil at the seafloor. In order to attain this reality, the crude oil would need to pass through additional separation stages. To predict how changing inlet conditions will affect the oil and water quality at the different stages of the separation more knowledge is needed about the compounds that affect the separation and how they interact, namely polar crude oil compounds like naphthenic acids and asphaltenes,.

This work will focus on the competitive adsorption at oil-water interface between naphthenic acids and asphaltenes. To do that the adsorption of these components will be studied by a powerful apparatus: a profile analysis tensiometer fitted with a co-axial capillary. This apparatus allows to study the competitive adsorption between several compounds and, also, determine the desorption of compound previously adsorbed.

This project is a part of the *SUBPRO* research centre, which is an 8-year SFI (center for innovation) at NTNU on subsea production and processing funded by the Norwegian Research Council and several industrial sponsors. The work will be performed at Ugelstad Laboratory, Department of Chemical Engineering.

Supervisor: Prof. Johan Sjöblom.

Co-supervisors: PhD candidate Are Bertheussen and Dr. Sébastien Simon.

21 COMPETITIVE ADSORPTION BETWEEN ARN TETRA-ACID AND ASPHALTENES AT OIL-WATER INTERFACES TO UNDERSTAND THE FORMATION OF DEPOSITS

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 shutdown. That is why it is important to determine the formation mechanism of these deposits.

In this project, the competitive adsorption at oil-water interface between ARN and other components present in petroleum crude oil such as asphaltenes will be studied by interfacial rheology, a powerful technique allowing to measure the rheological properties of interface. The experiments will allow to determine for which conditions, concentrations of ARN and asphaltenes, ARN is present at interfaces and able to form gel, precursor to deposists.

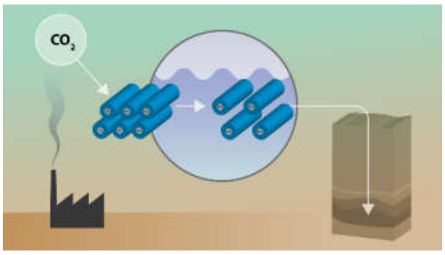
This project is a part of a research project between Ugelstad Laboratory and a major oil company. The work will be performed at Ugelstad Laboratory, Department of Chemical Engineering.

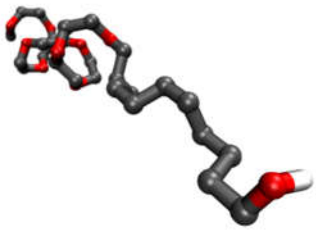
Supervisor: Prof. Johan Sjöblom.

Co-supervisor: Dr. Sébastien Simon.

Project offered by Associate Professor Kristofer G. Paso kristofer.paso@ntnu.no

22 Synthesis, Characterization, and CO_2 Capture with Liquid Crystals






This project is to make liquid crystals that will capture CO_2. The liquid crystals will capture, transport, and store CO2 in underground aquifers using a single solution (image left).

The student will begin with amphiphilic triblock copolymers consisting of polyethylene oxide blocks and polypropylene oxide blocks. These amphiphilic triblock copolymers already have terminal –OH groups. The student will modify the amphiphilic triblock copolymers with groups that will capture CO_2 (image center).

After the student makes the copolymer, the student will analyze the copolymer using NMR to confirm the modification synthesis is successful. (The new NMR in the biotechnology dept. will be used.)

After the student analyzes the copolymer, the student will check to see if the copolymer forms lyophilic hexagonal or lamellar liquid crystals using visual cross polarized observation, X-ray diffraction, and X-ray scattering.

The student will measure absorption of CO_2 in the liquid crystals using an already existing bench-scale apparatus. The CO_2 uptake will be compared with theoretical modelling performed at University of Bergen.

Finally, the student will study transport of CO_2 in liquid crystals using a rheometer (image right). The students data will be supplemented with external PVT data (storage of CO_2 in liquid crystals).

The student will be part of an exciting team including a Ph.D. student, post doctors, technicians, and professors, collaboration with the University of Bergen.

Pre-qualifications: Current master's student in chemical engineering or related discipline.

Projects offered by Professor Gisle Øye gisle.oye@ntnu.no

23 Injection of synthetic produced water into porous media

Produced water is a major co-product during crude oil production. The produced water typically contains dispersed and dissolved hydrocarbons and solid particles. If the produced water is going to be reinjected into a reservoir, the dispersed components must be removed to avoid blocking of the pores in the reservoir and subsequent loss in injectivity. The requirements of water quality prior to reinjection is not very well understood, but will depend on both reservoir and fluid properties.

The aim of this project will be to investigate the transport of dispersed components through simulated reservoir packs. A purpose-built cell will be used to follow the transport of oil drops by simultaneous pressure drop and optical detection. Important parameters to study will be the chemical properties of the emulsions as well as of the porous matrix.

Supervisors: Marcin Dudek and Gisle Øye

24 Removal of dispersed oil drops by gas flotation at elevated pressures

Produced water is a major co-product during crude oil production. The produced water typically contains dispersed and dissolved hydrocarbons and solid particles. If the produced water is going to be reinjected into a reservoir, the dispersed components must be removed to avoid blocking of the pores in the reservoir and subsequent loss in injectivity. Gas flotation is one water treatment method that is of interest when developing subsea production and processing facilities.

The aim of this project will be to investigate the oil removal efficiency of a purpose-built gas flotation cell that can be operated at elevated pressures. Important parameters to study will be the chemical composition of the involved phases (gas, oil and water).

The project is linked to the SUBPRO Centre for Research-based Innovation.

Supervisors: Marcin Dudek and Gisle Øye

25 Experimental investigation of the break-up and coalescence of crude oil drops in produced water

Produced water is a major co-product during crude oil production. The produced water typically contains dispersed and dissolved hydrocarbons and solid particles. The quality and treatment of produced water is influenced by the rates of break-up and coalescence of oil drops in the water, and understanding the main parameters affecting these processes is of fundamental interest.

The aim of this project is to investigate the formation of o/w emulsion under different mixing condition using a purpose-built mixing setup. The time dependent drop size evolution of the emulsions will be followed by laser diffraction analysis. Important parameters to study will include mixing speeds and chemical composition of the crude oil and water phases. A parallel project, in collaboration with Brian Grimes, will utilize the experimental results for modelling of the break-up and coalescence phenomena.

The project is linked to the SUBPRO Centre for Research-based Innovation.

Supervisors: Marcin Dudek and Gisle Øye

26 *MICROFLUIDIC INVESTIGATION OF DISPLACEMENT AND MOBILISATION OF OIL IN ENHANCED OIL RECOVERY PROCESSES*

Enhanced oil recovery (EOR) is the final stage in the recovery of crude oil from reservoirs. Much of the oil remaining in the reservoir prior to this stage is microscopically trapped in the pores by capillary action. The amount of remaining oil depends largely on the ratio between the viscous forces displacing the oil and the capillary forces trapping the oil. A microfluidic system is a lab-on-a-chip (here: reservoir-on-a-chip) device where micro-volumes of fluids can be controlled and studied in micro-channels or networks of micro-channels, and the fluid behavior often is followed by microscopy methods. This means that the technique is well suited for visualization and fundamental studies of phenomena governing oil mobilization and displacement at length scales where the capillary forces dominate

The aim of this project will be to develop microfluidic methodology for screening and optimization of mobilization and displacement of crude oil in EOR processes.

The project is linked to a VISTA program.

Supervisors: Marzieh Saadat and Gisle Øye

27 TRANSPORT OF HYDROLOGICAL TRACERS IN POROUS MEDIA

Tracers are used within hydrology to investigate flow paths, flow processes and residence times of watersheds and ground water. Different types of tracers can be used to provide information about hydrological parameters such as movement (direction and velocity) of ground water, potential contaminant in the water and the porosity and dispersivity of the porous matrix surrounding the ground water. Possible tracers include dyes, salts, stable isotopes and functionalized nanoparticles.

The aim of this project will be to develop methods for following transport of nanoparticle based tracers in porous matrices. An important parameter to study will be how the chemical composition of the porous matrix will influence the transport and retention of nanoparticle based tracers.

The project is a collaboration with Faculty of Civil Engineering and Geosciences, TU Delft.

Supervisors: Gisle Øye (NTNU) and Sulalit Bandyopadhyay (TU Delft)

28 THE EFFECT OF BIOCIDES ON O/W EMULSION STABILITY

Biocides are often added in produced water treatment facilities to control the bacterial growth. However, little is known about how the biocides may influence the stability of dispersed oil present in the produced water, and thereby how they affect the treatment efficiency of the water.

The aim of this project is to investigate how various biocides affect the stability of crude oil emulsions. Interfacial properties, drop sizes and creaming rates will be the most important parameters to study.

The project is linked to the SUBPRO Centre for Research-based Innovation and is a collaboration with Department of Geoscience and Petroleum.

Supervisors: Gisle Øye and Milan Stanko/Håvard Skjefstad (Department of Geoscience and Petroleum)

Projects offered by Associate Professor Brian Grimes, brian.grimes@ntnu.no

29 Development of a novel membrane separator for emulsions

Co-supervisor: Aleksandar Mehandzhiyski

Description: The separation of emulsions in crude oil processing is an important step to facilitate transport and sale of the final product. In many cases, a significant fraction of small water droplets remain in the oil after the first gravity separation step which can complicate subsequent transport and refinement processes without additional treatment. Traditional methods of using membranes for secondary emulsion purification are limited by the pressure drop required to drive fluids across the membrane. In this project, a novel membrane separator for emulsions that uses electrochemical separation mechanisms will be designed, manufactured, and tested. A prototype separator has been built and the student will test this prototype separator under a wide range of operating conditions to determine if the concept is feasible. Use of the device for the separation of water continuous emulsions will also be investigated. The student should determine the operating parameters of the prototype that facilitate separation. A background in transport phenomena and/or electrochemistry along with a desire to work in the laboratory and do some basic modeling is recommended.

30 Development of a transport enhanced dye sensitized solar cell (DSSC)

Description: Dye sensitized solar cells (DSSC's) are a promising technology for solar energy generation due to their cheap materials and ease of fabrication. However, the performance of DSSC's still needs to be improved in order to make them commercially viable. One limiting step in the performance of DSSC's is the transport of electrolyte between the cathode and anode in the cell. In this project, a novel design for a transport enhanced DSSC will be formulated, fabricated and tested. The student will build and test this new transport enhanced DSSC and evaluate its performance relative to conventional DSSC's and silicon based solar cells. A background in transport phenomena along with a desire to work in the laboratory and do some basic modeling is recommended.

31 Theoretical investigation of the break-up and coalescence of crude oil drops in produced water

Co-supervisors: Shamsul bin Ismail, Marcin Dudek, and Gisle Øye

Produced water is a major co-product during crude oil production. The produced water typically contains dispersed and dissolved hydrocarbons and solid particles. The quality and treatment of produced water is influenced by the rates of break-up and coalescence of oil drops in the water, and understanding the main parameters affecting these processes is of fundamental interest.

In a parallel project, in collaboration with Gisle Øye, experimental results for the break-up and coalescence of oil droplets in a water continuous emulsion under different mixing conditions will be produced. The experimental time dependent drop size evolution of the emulsions will be regressed to population balance model developed previously. It is recommended that the student should have good skills in computer programming and mathematics, particularly in differential equations.

The project is linked to the SUBPRO Centre for Research-based Innovation.

32 DEVELOPMENT OF A MODULAR GRAVITY SEPARATION MODEL

Co-supervisors: Christoph Josef Backi, Aleksandar Mehandzhiyski

The development of accurate models for gravity separators is essential for monitoring and model based control schemes if this technology is to be successfully and reliably employed in subsea production. In this project, a modular population balance model for gravity separation will be developed as a class object. This separation class object will subsequently be employed to generate models of continuous gravity separators at various levels of complexity with the primary focus of predicting oil content in the separated water.

It is strongly recommended that the student should have good skills in Matlab computer programming, with a strong desire to eventually learn object orientated programming and C/C++. Additionally, successful comprehension of the transport phenomena course and strong skills in mathematics, particularly in differential equations, are highly recommended.

The project is linked to the SUBPRO Centre for Research-based Innovation.

33 COARSE GRAIN MOLECULAR SIMULATIONSS OF COALESCENCE

Co-supervisor: Aleksandar Mehandzhiyski

Coalescence is a complex, multi-scale process that is one of the main physical phenomena driving gravity separation of crude oil process streams. Despite a long history of study, the molecular phenomena involved in the coalescence process are empirically described or oversimplified for crude oil systems. In this project, a course grained molecular simulation will be developed to bridge the spatial and temporal gap between full atomistic molecular simulations and continuum film drainage models. The primary focus with be to predict coalescence times in water continuous emulsions.

It is strongly recommended that the student should have good skills in computer programming and scripting in Linux.

The project is linked to the SUBPRO Centre for Research-based Innovation.

34 MOLECULAR SIMULATIONS OF IONIC LIQUIDS IN SUPERCAPACITORS.

Co-supervisors: De Chen, TBD

Supercapacitors are a promising technology for delivering electrical energy with short charging times. The performance of super capacitors is strongly linked to the molecular orientation of the ionic liquids (IL's) in the porous electrodes. Molecular dynamics (MD) simulations have been successfully applied for the study of supercapacitors and a model developed in house. In this project, the student will assist a post-doc to learn and perform atomistic MD simulations to obtain the densities and spatial distributions of the IL inside a negatively charged porous electrode over a large range of pore sizes, IL composition, and surface charge.

It is strongly recommended that the student should have good skills in computer programming and scripting in Linux.

Environmental Engineering and Reactor Technology

Projects offered by Professor Jens-Petter Andreassen, jens-petter.andreassen@ntnu.no

35 Crystallizaton of nickel sulphate for use in car batteries

Co-supervisors: Ina Beate Jenssen (NTNU) and Oluf Bøckman (Glencore)

Electric cars are one of the contributions to a green shift in the transport sector. The batteries in electric cars contain several metals, among them nickel. Nickel can originate from metallic nickel, nickel sulphate or other nickel compounds. Glencore Nikkelverk in Kristiansand is among the world leading producers of metallic nickel and the company is now considering, in addition to their electrolysis process, to produce a nickel sulphate salt by crystallization from one of their side streams.

The project assignment is to evaluate different processes for crystallization of nickel sulphate based on a literature survey and to perform an experimental crystallization study based on a feed containing 3-5 g/l Na, 0,5 g/l Mg, 40 g/l Ni with the corresponding level of sulphate and chloride at a pH of about 2. Temperature, pH and supersaturation should be varied in order to establish the effect on yield, size and purity of the crystals.

36 Tailoring the growth of multifunctional nanoparticles (NPs) for environmental applications.

Recent years have seen an increasing demand of smart nanomaterials in diagnosis, therapy, quality control, resource management among others that are capable of carrying out several functions simultaneously with precision and accuracy. In most such applications, integrating several functionalities into a single nanoconstruct is desired, leading to the formation of smart materials. In essence, a single nanoconstruct might be able to remain in circulation for long, possess optically detectable properties (tracking), bind to a specific molecule, undergo a detectable change in properties and so on. Majority of such constructs require optimization of synthesis and encapsulation steps to achieve unprecedented functions.

In this project, several methods would be used to form stimuli-responsive nanogels coupled with inorganic NPs that can be triggered to release a cargo of interest in a controlled manner. Primary focus will be on optimization of system parameters in order to modify the physico-chemical properties of the constructs. Following an optimized synthesis protocol with detailed understanding of the growth mechanisms, different biomolecules like DNA, proteins will be encapsulated to estimate loading properties of these nanoconstructs. In the final part of the project, the multifunctional NPs would be evaluated for different environmental applications that stem from tracing of contaminants in water lines to scavenging of micro-organisms in water streams.

The project will be carried out in collaboration with TU Delft, Netherlands, with a possibility of exchange stay, if there be need.

Co-supervisor: Sulalit Bandyopadhyay (TU Delft/UNESCO IHE, IKP)

Projects offered by Associate professor Liyuan Deng, liyuan.deng@ntnu.no

37 Preparation of hollow fiber membrane module for CO_2 capture using membrane contactor (in 3GMC project)

Membrane contactors represent a viable solution to reduce amine evaporation in post combustion CO_2 capture processes. Membrane contactor tests have been performed for dense AF2400 membranes and thin composite membranes (AF2400 coating on porous polypropylene, PP), showing promising results. The Teflon AF polymer series has been found to be chemically compatible with various solvent systems and it has been characterized in terms of amine and CO_2 permeation. However, the hollow fiber configuration is needed for further scale-up of the technology. Therefore hollow fiber membrane module must be prepared, where commercially available PP fibers are coated with the AF2400 thin layer. Currently, a simple procedure is used for the coating, which allows the preparation of modules with an interface area up to 35 cm^2. However, larger interface areas are required to test the contactor in conditions that are closer to the real separation process.

The tasks of the project can be summarized as:

1) Implementation of a coating procedure to fabricate thin composite hollow fiber membranes and preparation of membrane modules with a membrane area larger than 100 cm^2;
2) Investigation of the separation performance of the module in a membrane contactor apparatus.
3) Evaluation of the amine evaporation through the membrane layer.

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

38 Membrane fabrication and characterization for dehydration of triethylene glycol

(This project is bound to the summer job in the SUBPRO project)

Natural gas (NG) dehydration is an important step to reduce problems (i.e., hydrate formation) in the NG transport. Currently, the most used dehydration technology in the natural gas industry is absorption/desorption in triethylene glycol (TEG), but its implementation subsea presents several constructing limitations. A closed loop membrane contactor offers a more feasible solution, thanks to the more compact design. Process simulation investigation are currently ongoing, trying to verify the feasibility of the process, but a lack of experimental data limits the analysis of the desorption process. In this view, the present project focuses on the practical fabrication and characterization of membranes for TEG dehydration. An initial investigation showed that hydrophobic membranes can be suitable for this operation, but other materials may be considered.

The tasks of this work are:

1) Synthesis and preparation of nanocomposite membranes with specific TEG-H_2O selectivity;
2) Morphological characterization of the membranes;
3) Experimental testing of the separation performance of the synthesized membrane performance for the TEG dehydration under different temperatures.

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

39 Development of high performance cross-linked polyethylene glycol (PEG) based mixed matrix membranes for CO_2 separation (in NANOMEMC[2] project)

Membrane gas separation has received considerable research attention for CO_2 capture from flue gas and natural gas sweetening due to their advantages including operation flexibility, easiness to operation and small footprint. Membranes containing polyether groups (PEG) are of particular interest for CO_2 removal owing to the strong interaction between the quadripolar CO_2 and the polar ether bonds. However, the performance of pure PEG membranes suffers significantly from its high crystallinity, as the crystalline regions within the membrane are not gas permeable. Cross-linking of the PEG can effectively reduce the crystallinity of the polymer and thus improve the gas permeability.

The present project includes three tasks:

1) Optimization of PEG cross-linking conditions (e.g., reactant molar ratio, reaction time, reaction temperature);
2) Screening of proper nano-fillers as additives into the PEG polymeric matrix;
3) Investigation of the gas separation performances of the resulted membranes at different temperature and relative humidity conditions.

Supervisor: Assoc. Prof. Liyuan Deng, Co-supervisor: Dr. Zhongde Dai

40 Fabrication of nanocellulose based facilitated transport membranes for CO_2 capture (in NANOMEMC[2] project)

Facilitated transport membranes are very promising for CO_2 capture from flue gas, as the CO_2 permeance and selectivity can be simultaneously improved through reversible reactions between CO_2 and reactive carriers. Recently Nanocellulose has been used as nano materials in gas separation membranes. Very high selectivity value for both CO_2/N_2 and CO_2/CH_4 have been obtained, but with rather low CO_2 permeability. In the present work, nanocellulose is to be added to polyallylamine (PAA) matrix to enhance the CO_2 flux across the membrane. The amino groups in PAA provides CO_2 reactive carriers, and thus the CO_2 transport follows the facilitate transport mechanism. The project tasks include:

1) Fabrication of PAA-nanocellulose thin-film-composite membranes on a porous support (e.g., polysulfone);
2) Invesitgation of CO_2 separation performances using CO_2/N_2 mixed feed gas in a wide range of humidity conditions at low temperature (35 °C) and low pressure conditions (1.7 bar).
3) Investigation of other physicochemical properties of the membranes, such as thermal stability, water uptake, morphology and mechanical properties.

Supervisor: Assoc. Prof. Liyuan Deng, Co-supervisor: Dr. Zhongde Dai

41 Hybrid membranes for CO_2 capture (in NANOMEMC[2] project)

Global climate change expedites the need for economically feasible and less energy-intensive processes for CO_2 capture. Facilitated transport membrane-based processes feature as a potential alternative to conventional amine-based absorption processes due to the membrane's high permeability and selectivity towards CO_2. Recent studies have exposed that the use of nanomaterials with high affinity towards CO_2 inside existing polymer membranes can further enhance the transport properties of the membrane. Performance of such 'hybrid' membranes (nanocomposites) can be tailored by exploiting properties of individual components (nanofillers and polymer) and the properties that arise due to their interactions.

Use of nanocellulose fibrils and graphene oxide-based nanomaterials as nanofillers in polymeric matrices will we explored in this project. The nanofillers that are supplied by the project partners can be used as received. However, modifications of nanofillers prior to their incorporation in polymer matrix can also be delved into. The tasks of the project include:

- Fabrication of hybrid membranes in the form of self-standing films or thin layer composites through various techniques
- Testing of membrane permeation properties under different humidity conditions
- Fine tuning of membrane performance with nanofillers
- Elucidation of relationship between properties of nanofillers and performance of nanofiller embedded hybrid membranes. This can be accomplished by studying properties of hybrid membranes using various characterization techniques available at the group facility, and Nanolab if necessary

Supervisor: Assoc. Prof. Liyuan Deng, Co-supervisor: Phd student Saravanan Janakiram

42 FABRICATION OF IONIC LIQUIDS GRAFTED MEMBRANE FOR CO_2 SEPARATION (IN POLYMEM PROJECT)

Poly(ionic liquid)s (PILs) have been considered as a promising new membrane material for CO_2 separation. However, the permeability of PILs membrane is usually low due to the strong attraction between cations (or anions) in polymer chains and free anions (or cations). Recently, the modification of PIL membranes are mainly focused on molecular design and blend with various ILs. In this project, a new approach to improve the permeability of ILs-based membranes is proposed. Selected ILs will be grafted onto the surface of highly permeable bulk membranes to improve the selectivity of the membranes.

The scope of this work can be specified as follows:

1) Fabrication and screening of highly permeable bulk membranes (ROFs, poly[1-(trimethylsilyl)-1-propyne] and poly[1-(trimethylsilyl)-1-propyne]);
2) Surface grafting of [MATMA][Gly] on the surface of selected membranes by UV grafting;
3) Investigation of CO_2 separation performances of the ILs grafted membranes;
4) Characterization of the ILs grafted membranes by using FT-IR, SEM and AFM, TGA and DSC.

Supervisor: Assoc. Prof. Liyuan Deng, Co-supervisor: Phd student Jing Deng

PROJECTS OFFERED BY ASSOCIATED PROFESSOR HANNA KNUUTILA, HANNA.KNUUTILA@NTNU.NO

43 CO2 SOLUBILITY, HEAT OF ABSORPTION AND VISCOSITY OF GLYCOL + MEA HYBRID SOLVENTS

The student should run CO2 heat of absorption analyses with hybrid solvents containing MEA, water and glycols (MEG, DEG and TEG) employing either the CPA202 or the CPA122 in the basement of K4. VLE curves will be obtained during the same procedure. If possible, the influence of stirring velocity should be assessed at least for one solvent formulation. Additionally, as viscosity is an important parameter related to absorption efficiency, experimental viscosity data for the lean solvents should be produced using the viscometer. This experimental series will be useful for providing insights regarding the feasibility of employing such absorbents in industrial applications

Supervisors: Prof. Hanna K. Knuutila and Ricardo R. Wanderley

44 ETHYLENE OXIDE PRODUCTION FROM CO2: SIMULATION AND STATE OF THE ART REVIEW

In this work, the student will review the production pathways for ethylene oxide production. The state of the art process will be simulated in, for example, Aspen plus and regarded as the base case. In addition, the production of ethylene oxide from CO2 will be simulated and compared with the base case. Identification of the energy requirements and energy sinks will be one of the focus of the study.

Supervisors: Prof. Hanna K. Knuutila

45 IDENTIFICATION OF POTENTIAL PROMOTERS FOR CO_2 ABSORPTION PROCESS

An important part in the work of reducing the energy associated with amine-based absorption process, for CO_2 capture, is the selection of a solvent system with better performance than the benchmark solvent 30wt% MEA. A solvent system that has received great attention is the blended system 2-(Diethylamino)ethanol (DEEA) + 3-(Methylamino)propylamine (MAPA) + H2O. The blend combine the high reactivity from the diamine MAPA and the low heat of absorption from the tertiary amine DEEA. However, as MAPA is a toxic and volatile amine, it is desirable to find a substitute that is more environmental friendly.

In this work, the aim is to identify potential primary/secondary amines that can be used to promote DEEA. The amine solvents will be studied using a double stirred cell reactor, which allows for calculation of both absorption rate and absorption/desorption capacity.

Supervisors: Prof. Hanna K. Knuutila and Ida M. Bernhardsen

46 DEGRADATION OF ABSORBENT SYSTEMS

Alkanolamines are widely used as solvents for acid gas removal because many of them react fast with CO2/ H2S and they have high absorption capacity. One major problem using amines is degradation which causes additional operating costs related to solvent losses, corrosion of process equipment, fouling, foaming and the potential effects that the degradation products may cause to the environment.

This project work is perform a systematic study investigating the degradation of amine blends and hybrid solvents. The work will be experimental. Degradation compounds will be identified using different analytical instruments, IC and LC-MS. The task will be to perform a systematic study on the influence of amine concentration and water content on degradation in the presence of acid gases. The autumn project is planned to continue to an MSc thesis, but not necessarily in the same area.

Supervisors: Prof. Hanna K. Knuutila

47 MEASURING PHYSICAL SOLUBILITY OF N2O/CO2 IN SEVERAL SOLVENTS

In this work, the student will measure the solubility of CO2 and N2O in several solvents including Monoethylene glycol (MEG), tri-ethylene glycol (TEG), MEA, MDEA, and aqueous mixtures of these solvents at 5 different temperatures. The measurements will be performed in an equilibrium apparatus previously used for this kind of measurements. The student will also measure the density and viscosity of these solutions at atmospheric conditions and at the experiments temperatures.

The results will serve as a validation for a computational model based on Monte Carlo simulation.

Supervisors: Prof. Hanna K. Knuutila

PROJECT OFFERED BY PROFESSOR JANA JAKOBSEN, JANA.P.JAKOBSEN@NTNU.NO

48 FACILITATING DEPLOYMENT OF CARBON CAPTURE TECHNOLOGIES THROUGH MODELING AND SIMULATION: TESTING THE CCSI TOOLSET DEVELOPED BY NATIONAL ENERGY TECHNOLOGY LABORATORIES IN THE US

One of the most critical problems the earth is currently facing is the global warming caused by increasing emissions of greenhouse gases. Today, there is a common international understanding that the emissions of greenhouse gases need to be reduced. Carbon Capture and Storage (CCS) is believed to be the most important measure to achieve the reduction of CO_2 emission from power production and industrial sources. However, the pace of deployment of CCS technologies is too slow.

National Energy Technology Laboratories (NETL) in the US initiated Carbon Capture Simulation Initiative (CCSI). The aim of the initiative is to accelerate the commercialization of carbon capture technologies from discovery to development, demonstration, and ultimately the widespread deployment to hundreds of plants. A state-of-the-art, comprehensive, integrated

suite of validated science-based computational and simulation models was developed (CCSI Toolset) and is now available for testing.
The proposed project will focus on testing the CCSI Toolset specifically the models for 3 types of CO_2 capture technologies: absorption, membrane, and adsorption. The main tasks will be: getting familiar with the user interface, gaining insight into the overall structure of the toolset as well as the design basis and the assumptions for the particular models, setting up a suitable test case and evaluating the tool performance, providing an overview of advantages and limitations of the toolset.

Qualifications/prerequisites:

- Interest in development of environmentally friendly technologies
- Interest in modeling and simulation of operational units
- Fundamental knowledge of fluid flow, heat and mass transfer, thermodynamics, and chemical reaction kinetics
- Basic knowledge of the principles of modeling and simulation in chemical engineering

PROJECTS OFFERED BY PROFESSOR HUGO A. JAKOBSEN, HUGO.JAKOBSEN@NTNU.NO

49 REVIEW OF NON-NEWTONIAN FLUID STRESS MODELS APPLIED IN (REACTOR) MODELING

In chemical and biochemical reactor technology the rheology of dense fluid suspensions in the bulk may become important for determining the process performance as well as the surface rheology of drops and bubbles in multiphase systems. These phenomena will influence on the transport phenomena and on the interfacial mass transfer in these units.

The project start out with a literature review to get an overview of the fundamental models and the existing applications of such models in reactor technology.

The fundamental theory will then be applied to describe fluid particle coalescence modeling and implementation. The project has many interactions with the second project on film drainage modeling and collaboration can be advantageous.

The project is intended to be continued in a master thesis.

Supervisors: Professor Jannike Solsvik and Hugo A. Jakobsen

50 FILM DRAINAGE BETWEEN COLLIDING DROPS AND COLLIDING BUBBLES

Understanding the evolution of liquid–liquid and gas-liquid dispersions requires an advanced knowledge of the main processes that control the distribution of the interfacial area, drop breakage which increases it and coalescence which reduces it. The coalescence efficiency depends on the ratio of two characteristic time scales:

— the contact time t_c which is mainly controlled by the external flow, and
— the drainage time t_d of the film thinning between drops until rupture by molecular forces.

In order to estimate t_d, film drainage must be modeled for the various situations encountered in industrial and environmental systems. Interfacial behavior and the conditions of approach and contact must be taken into account by suitable approximations of the initial and boundary conditions.

For liquid–liquid dispersions, models have been developed for gentle collisions of two spherical drops, i.e., for collisions for which the contact time is sufficient to allow drainage and rupture to occur. Various regimes of drainage can be distinguished depending on the mobility of the interfaces. Interfaces are said immobile when their tangential velocity is zero, partially or fully mobile when film drainage and inside drop flow are coupled by their tangential velocity at the interfaces, and fully mobile when there is no tangential stress at the interfaces.

In this project the derivation of the model by Klaseboer et al (2000) should be elucidated pointing out all model assumptions followed by a discussion of the validity of these assumptions. This is an extension of a previous project student work by Mathias Eng. The project will then extend this modeling framework aiming at developing a model with a more general surface rheology similar to the model proposed by Narsimhan (2016).

References:

Klaseboer, E., Chevaillier, J. Ph., Gordon, C., and Masbernat, O., Film Drainage between Colliding Drops at Constant Approach Velocity: Experiments and Modelling, Journal of Colloid and Interface Science **229,** 274–285, 2000

Narsimhan, G., Characterization of Interfacial Rheology of Protein-Stabilized Air-Liquid Interfaces, Food Eng Rev 8 (3) 367-392, 2016

This project is reserved as a master thesis project for Marco Piloni (marco1.piloni@mail.polimi.it), a visiting MSc student from Milano.

Supervisors: Professor Jannike Solsvik and Hugo A. Jakobsen

51 BUBBLE BREAKAGE – IMAGE PROCESSING AND PROGRAMMING

Gas-in-liquid dispersions play an important role in numerous industrial applications. The interface mass, momentum and heat fluxes between the gas and liquid phases are fundamental to optimize the performance of, for example chemical reactors such as the bubble columns. The interfacial mass, momentum and heat fluxes do not only depend upon the dynamic interaction between the phases, but also importantly relate to the interphase area. Phenomena such as bubble breakage and coalescence directly influence on the interfacial area. In the present study, the focus is placed on the bubble breakup phenomenon.

In this study we investigate the bubble breakup phenomenon in detail using high-speed imaging, which allows high spatial and temporal resolution of the breakage event. An infinitely dilute system is considered to avoid noise from other bubbles in the images. The breakage cell consists of a rectangular tank where the bubbles are injected in the bottom and with nozzles at the top of the tank. An example of an images sequence of a binary bubble breakup event is shown in the Figure.

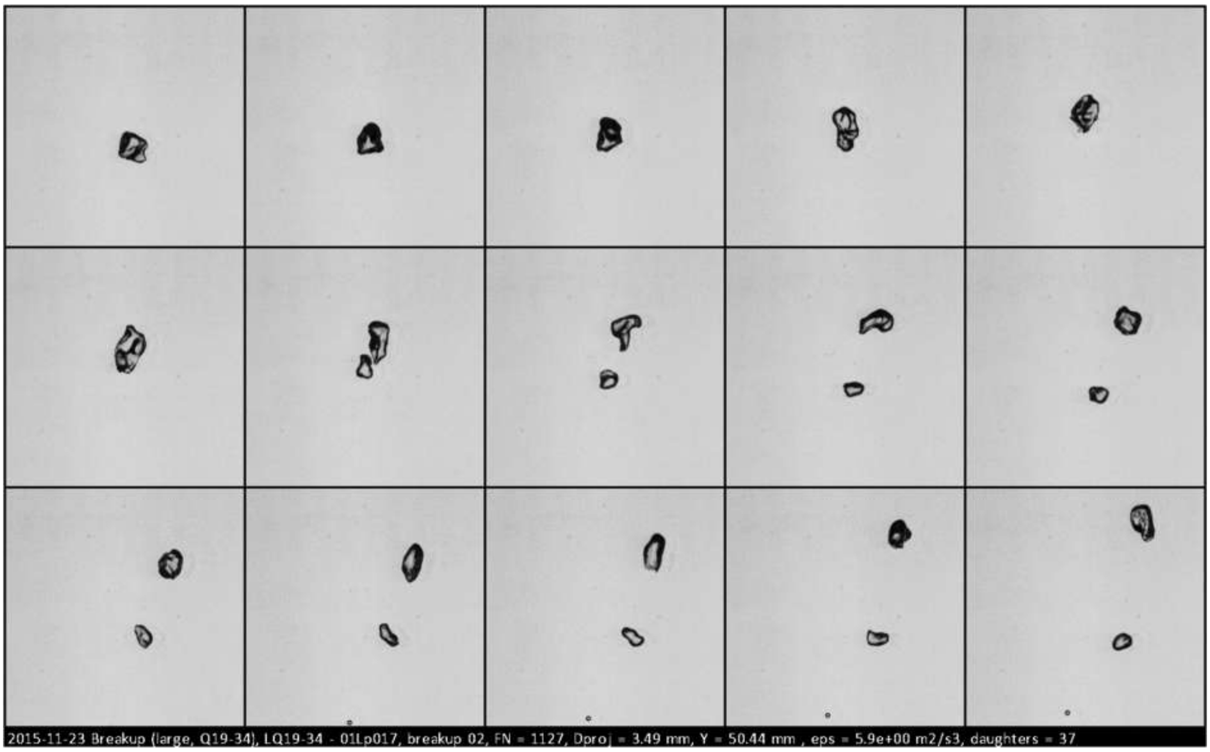


FIGURE: IMAGE SEQUENCE OF A BINARY BUBBLE BREAKUP EVENT.

The detailed study of bubble breakup events allows us to determine the breakage time, breakage probability, number of daughter bubbles, and daughter size distribution. Such information on the bubble breakup phenomenon is important for validation of the breakup models in the literature as well as for the further development of the mathematical model framework for breakage. The bubble breakage phenomenon is still not well understood and the existing models give contradictory predictions.

A high number of bubble breakage events must be evaluated in order to have a statistical representative set of data. In the present work, a program will be developed in MATLAB for image analysis to support the handling of a large number of images to be analyzed.

The relevant student must have good skills in programming (MATLAB) and mathematics/statistics.

The project is intended to be continued in a master thesis.

Supervisors: Professor Jannike Solsvik and Hugo A. Jakobsen

52 BUBBLE RISE VELOCITY EXPERIMENTS

Knowledge on bubble motion is required for the accurate prediction of gas-liquid two-phase flows in, e.g., the bubble column reactor. In this work we will develop a model for the drag coefficient of single bubbles under different fluid properties and bubble diameters.

This task involves both experimental work, data treatment and mathematical modeling.

The experimental part uses high-speed imaging to study single bubbles rising in a pipe. For statistical reliable results, a high number of videos must be recorded and analyzed. To simplify the work with the video analyses, the MATLAB Image Processing Tool will be used. The bubble rise data should be analyzed by statistical tools. Mathematical modeling and parameter fitting based on the resulting data should result in a model for the drag coefficient.

The relevant student must have interest in
- experimental work (high-speed imaging)
- MATLAB (image processing)
- statistics (error analysis and parameter fitting)
- mathematical modeling

The project is intended to be continued in a master thesis.

Supervisors: Professor Jannike Solsvik and Hugo A. Jakobsen

53 Gas-Liquid Mass Transfer Limitations in Bioreactors

Review of model and correlations for the liquid side gas-liquid interface mass transfer coefficient and experimental setups for measuring the mass transfer coefficient as a function of bubble size.

The aim is that an optimal design of an experimental setup may be proposed. A suitable system comprising a liquid and a gas must be selected to ensure a sufficiently large physical absorption rate to determine the mass transfer coefficient with sufficient accuracy (20-30% uncertainty). The proposed setup should be designed, build and experiments should be performed. The bubble size range investigated should be in the range 1 mm downwards to 1 micrometer if possible.

A Lagrangian model describing the mass transfer from a single bubble following the trajectory of the bubble through the setup tube. This model will be used to fit the empirical parameters in a suitable mass transfer correlation to the experimental data.

The accuracy of the mass transfer coefficient must be determined.

The project is intended to be continued in a master thesis.

Supervisors: Professor Jannike Solsvik and Hugo A. Jakobsen

Projects offered by Proffessor Magne Hillestad, magne.hillestad@ntnu.no

54 REN-BTL: Integration of renewable production of hydrogen in current Biomass-to-Liquid Biofuels production systems

The REN-BTL project aims to significantly improve the carbon efficiency, and hence the economic and environmental performance, of liquid biofuels production by integrating efficient and renewable production of H_2 utilizing excess waste heat from the biomass to liquid biofuels conversion process.

Tasks (bør endres ettersom hvor mye Eirik gjør ferdig)

- Optimal design – staging and sizing of equipment
- Select the best CO_2 capture process from syngas at high pressure
- Optimal process configuration
- (Optimal operating conditions, recycle and purge)
- Heat integration
- Modelling of SOEC (Solid Oxide Electrolysis Cell)

REN-BTL is a project supported by the Norwegian Research Council with international participation.

Supervisors: Magne Hillestad and Erling Rytter

55 MATHEMATICAL MODELING AND MODEL FITTING FOR FISCHER-TROPSCH KINETICS

Reaction kinetics model structures will be identified from published laboratory data. Parameters will be estimated and uncertainties of the estimates will be calculated. The task requires use of Matlab or Python programming. Some training in Matlab or Python programming and regression methods for model fitting will be given. The FT kinetics includes description of the overall consumption rate of reactants and selectivity of products. The selectivities may be described by one or more growth factors and additional reactions.

Tasks:

- Literature review of models and published data
- Model and simulate the experimental setup.
- Formulate a consistent kinetic model that can be identified from measurement
- Estimate kinetic parameters and calculate the confidence interval of parameters
- Model discrimination

Supervisor: Magne Hillestad and Erling Rytter

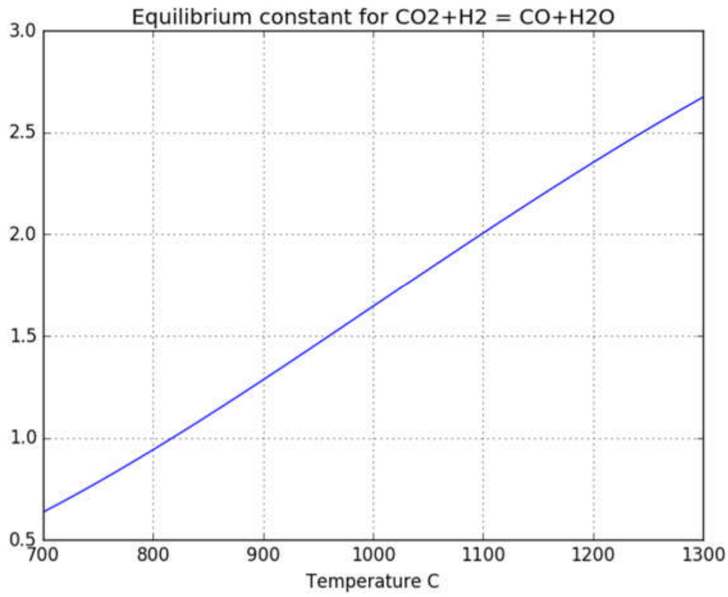
56 A FISCHER-TROPSCH SLURRY BUBBLE COLUMN REACTOR MODEL

A dispersion type reactor model of a slurry bubble column reactor is to be formulated and programmed in Matlab. The model will later be implemented as an extension in Hysys.

Supervisor: Magne Hillestad

57 HIGH TEMPERATURE REVERSED WATER GAS SHIFT REACTION

The reversed water gas shift reaction $CO_2+H_2 = CO + H_2O$ is to be studied experimentally. The feed gas is a synthesis gas from a biomass gasifier at equilibrium, where extra CO_2 and H_2 will be added to improve overall carbon efficiency of a BTL process. High temperature water gas shift catalysts are active at 310-450 C with Fe_2O_3/Cr_2O_3 catalyst. This catalyst will not withstand temperatures above 550 C.



The need for a catalyst is reduced at very high temperatures. The following item will be explored:

- How fast will the reaction go to equilibrium at temperatures in the range 800-1300 C with or without extra surface areas? The surface area may be metal or ceramics, with or without a catalyst component.

Supervisors: Magne Hillestad and Erling Rytter

Process Systems Engineering

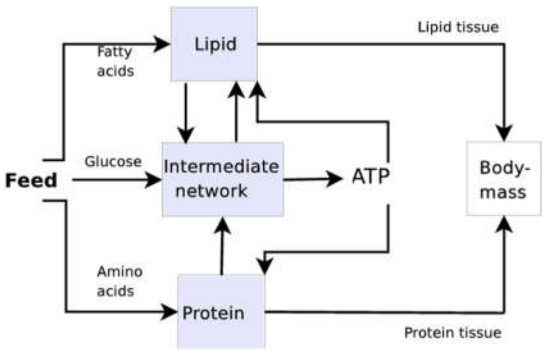
Projects offered by Professor Nadav Bar, nadi.bar@ntnu.no

58 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.

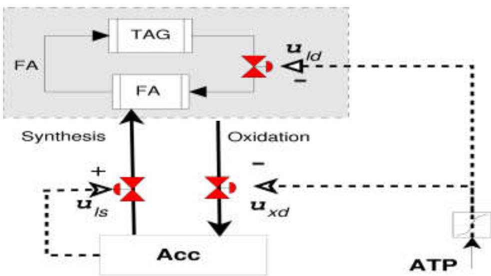
The main goal of this project is to optimize the integration method of the model, using a combination between a constant time-step and Matlab's ODE time variable solvers (ode45, ode15s). The project is interesting since it attempts to give a practical, industrial, applied solution to a theoretical model. 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: Nadav S. Bar nadi.bar@ntnu.no

Collaboration: Engineering Cybernetics, SINTEF Havbruk, Biomar AS.

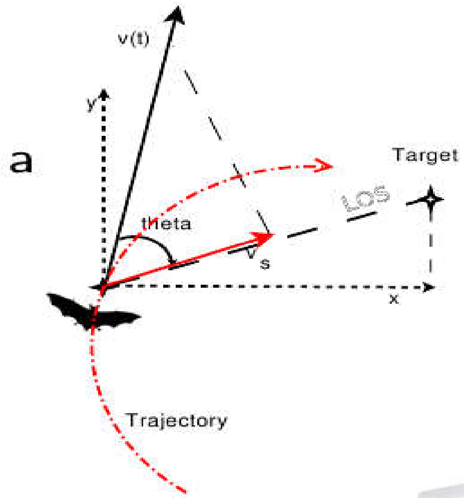


59 Modeling and simulations of bat sensori-motion control (Systems biology).

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. defense), 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).

The main goal of the project is understand the sensory system of the bat, and how the bat controls the head movement in relation to its body in order to achieve optimal sensory sight with the target. We need to analyse our lab data, develop a simple model and simulate it.



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

Benefits: Any technology company that works with signals, sonar, drones, subsea, Autonomous Underwater Vehicles (AUVs), and Unmanned aerial vehicles (UAVs) will be interested in your skills.

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

Main Supervisor: Nadav S. Bar.

Co-supervisor: Dr. Yossi Yovel, Bat lab, Israel.

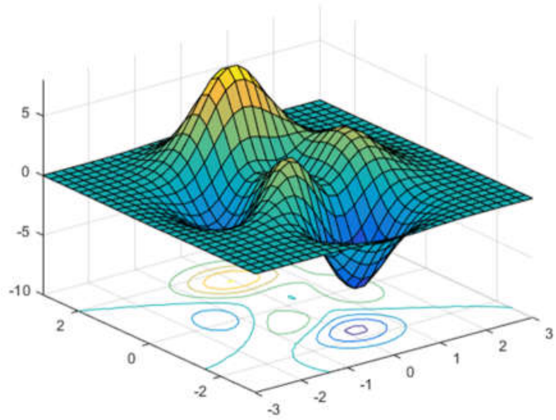
60 PARAMETER ESTIMATION OF STATE SPACE MODELS USING PARALLEL PROGRAMMING.

Most of the model we develop in genetic regulatory networks or in bio-chemical networks contain several parameters that we either cannot measure directly by experiments, or that are too expensive to measure. Some parameters have been measured before but these measurements are not accurate enough and therefore are not useful. In fact, the problem exists in biology, physics], economy, process, environmental modeling, and many more fields. We have more parameters than we can measure.

There are several methods to estimate such model parameters. But these methods require large computational resources, including parallel programming in C or Matlab, to distribute the computational load across thousands of CPUs.

We wish to develop a toolkit (a small matlab toolbox) that can estimate 3, 4, 5 model parameters and more simultaneously. You will develop functions and programs in matlab, programs that search from a large parameter space the right parameter by sophisticated tools and by parallel programming in NOTUR.

Benefits: you will learn MPI parallel programming that is highly desired today in the industry and computer science companies. You will learn to develop search algorithms including Branch and Bounds, genetic algorithms (for a search, nothing to do with biology), search trees, and parameter optimization. All these tools are highly useful in the academy and are increasingly needed in the industry, in small and large companies.



Main supervisor: Nadav Bar.

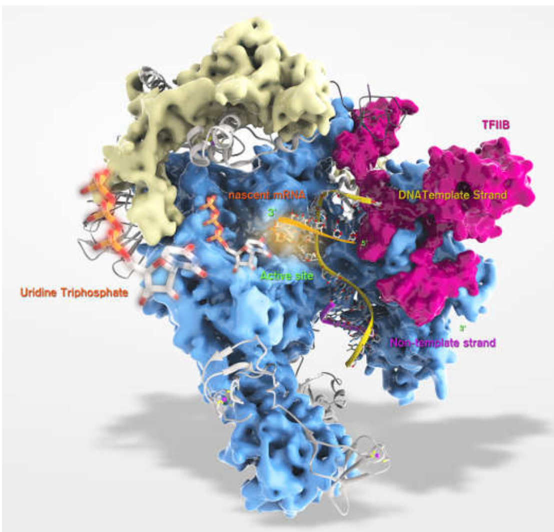
61 Simulations and Analysis of Model of RNA Polymerase Motion on the DNA

Our group has developed a dynamic model that simulates the motion of RNA polymerase (RNAP), an enzyme that mediate RNA synthesis from the DNA nucleotides. The process is very heavily controlled by different factor.

The objectives are to simulate the model, and understand the dynamic. We want to explore the behavior of the RNAP and how it leads to abortive initiation, the process where it stops synthesizing RNA and disassembles. Simulations and analysis will be conducted in Matlab. This exciting project and thesis will put you in the very cutting edge knowledge of microbiology and gene regulation mechanisms. Good results will most likely lead to publications and conference travels.

Benefits: you will learn how to simulate and analyze complex processes with simplified models using available data. This skills are very useful in the industry and academy.

Supervisor: Nadav Bar, NTNU



PROJECTS OFFERED BY PROFESSOR HEINZ PREISIG, HEINS.PREISIG@NTNU.NO

62 AN APPLICATION FOR MATERIAL PROPERTIES

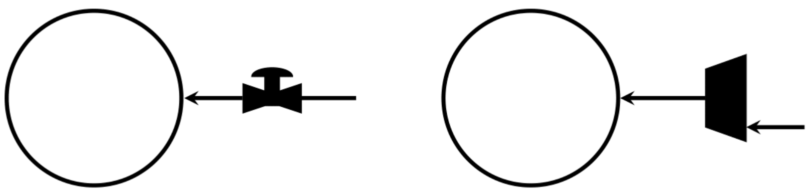
We are building a new modelling tool expanding on three previous generations of modelling tools, specially tailored for generating dynamic models for chemical processes, which are defined as functions of physical and material properties.

This project aims at implementing an application that provides an interface for requesting physical and material properties. This will involve:

- Analysing the properties of the dynamic process model and determine which properties can be requested from the material model software.
- Provide knowledge to the user on which information is missing in order to provide the material properties.
- Feed the material software with the properties it requires and broadcast the results dynamically back into the model.

The material model software is running and we are using it in a variety of ways. It would be very useful to build an interface that enables for interactive use of what the core of the software can generate. This interface could have the form of an application that can go along the modelling tool.

The application will be developed alongside a case study on the filling and discharge of a hydrogen storage tank as illustrated below. Each of the tanks can be filled or discharged, and the internal energy of the tank can be modelled using the five alternative set of variables.



i) $U = U(S, V, N)$ ii) $U = U(S(T, V, N), V, N)$ iii) $U = U(T, V, N)$ iv) $U = U(T, V, \mu)$ v) $U = U(T, p, N)$

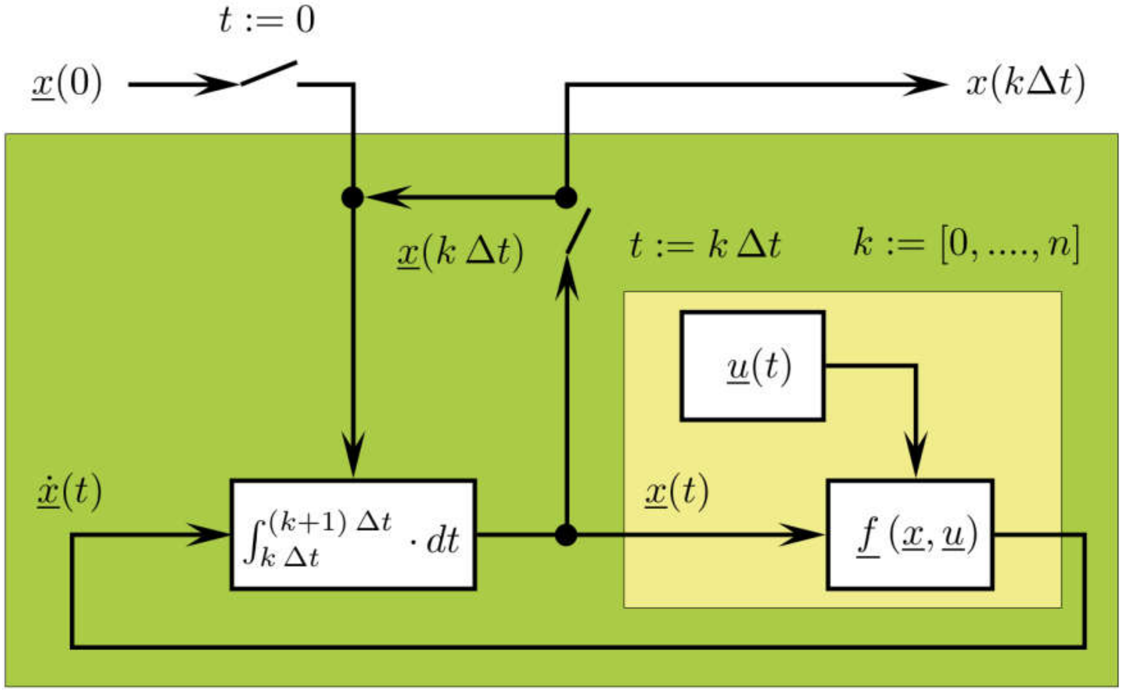
This project is a good opportunity refresh the thermodynamics and at the same time learn more on modelling and programming.

Supervisor and daily contact: Heinz A Preisig and Tore Haug-Warberg
Co-supervisor: Arne Tobias Elve

63 BUILDING A DYNAMIC MODEL SIMULATOR

We are building on a new modelling tool expanding on three previous generations of modelling tools. The modelling tool implements a step-wise approach to modelling as it is being taught in Process Modelling and the Systems Engineering course.

The objective of this project is to generate a dynamic model simulator, as illustrated in the included figure, that converts a defined model into executable program code.



The key to the construction of a dynamic model simulator is to map the algebra and the algorithmic part of a problem into code and how to do this automatically.

An excellent opportunity to learn more about modelling and programming.

Prior knowledge: None particularly, but the student should like to work with formal definitions, mathematical models, and programming in general.

64 Visual Modelling

We are building a new tool expanding on three previous generations of modelling tools. The objective of this project is to provide a high-level modelling tool for generating executable program code.

The executable program code can be in whatever language and can either be executed as a standalone or it can be integrated into existing software tools, such as gProms or other simulation environments.

The software builds on a graph representation of the processes, adds the “chemistry”. A “theory” module provides the basic descriptions, as the balance equations and, where appropriate alternative transfer specifications, kinetic laws, material descriptions and the like. The “theory” module is designed using a tool, which implements a simple, tailored language. The project aims at enhancing and partially substituting the current chemical engineering simulator software.

Prior knowledge: None particularly, but the student should like to work with formal definitions, mathematical models, and computer languages in general.

Projects offered by associated professor Tore Haug-Warberg, tore.haug-warberg@ntnu.no

65 *Characteristic time constant of coal fired furnace*

Full title: The characteristic time constant of an unsteady state coal or gas fired furnace buried in moist sand having a moving boundary of evaporated water

Background: The operation of small smelters for iron in particular, but also copper is troubled by the fact that the devices are in general not run at steady state, but over short periods of time which makes the dynamics of the furnace a key factor in the operational characteristics of the smelter. The chemistry of a smelter is quite (or actually very) complex and has been the subject of countless reports and academic publications, but even when keeping the chemistry out of the discussion, and focusing only on the time constant of the furnace from a thermodynamic point of view, there are unknown issues.

Goal: Continue the project work of Stud. techn. Garmann from 2016 (who has continued the work as a Master of Science project in 2017). The student can either take over the existing code and implement a more detailed chemistry including reaction kinetics, or take a more theoretical approach and look at different numerical discretization schemes and suggest more realistic geometries.

Prior knowledge and experience: The student must show interest in programming and numerical mathematics, and be motivated to read up on matrix calculations in general and eigenvector analysis in particular..

66 *A Lua Parsing Expression Grammar for exporting Markdown to HTML and LaTeX*

Full title: Implementing a Parsing Expression Grammar in the Lua programming language for parsing Markdown text into HTML and LaTeX.

Background: Writing blogs, manuals, reports and other documents with simple structure, but which at the same time should be esthetically pleasing and of technically high quality, is a a non-trivial issue. In the last decade or so the increased use of internet as a platform for professional discussion forums, there has been a marked interest into defining simple yet quite powerful input languages of which Markdown was the first. Many derivatives of Markdown have been suggested, but so far none is significantly better than the others. Which means there is still room for doing groundbreaking work...

Goal: The ultimate goal is to export Markdown text into HTML and LaTeX, but the parser must come first. Building a parser is a nice introduction to a very exiting field of computer science, namely that of language construction, ontologies, and automatic model generation (the link between these topics and the parser is not so clear at first, but it becomes very visible after a while).

Prior knowledge and experience: None particularly, but the student should like to work with formal definitions, mathematical models, and computer languages in general.

67 Defining a novel process systems modeling language using Parsing Expression Grammars in Lua

Full title: Defining a novel process systems modeling language for capturing physico-mathematical models using Parsing Expression Grammars in the Lua programming language

Background: The implementation of physico-mathematical models can, theoretically, be handled using templates that describe different parts of the model (such as physical units, parameters, variables, and mathematical expressions) and then combined to form the complete model. Note: An important key aspect is that the model should (must) be logically consistent to reduce hard-to-find semantic bugs. However, in order to make these templates adaptable and feasible for different purposes of the modeling activity, this project aims at providing a template mechanism by paring string expressions of equations in the model description into Lua templates, and then further translate Lua templates into executable code for the targeted language which could be Matlab or C or whatever.

Goal: The resulting parser shall be a portable product such that it can serve as a front end to our in-house simulator environment TOBOsim, or a commercial product like e.g. gProms.

Prior knowledge and experience: The student must know how to program in Python.

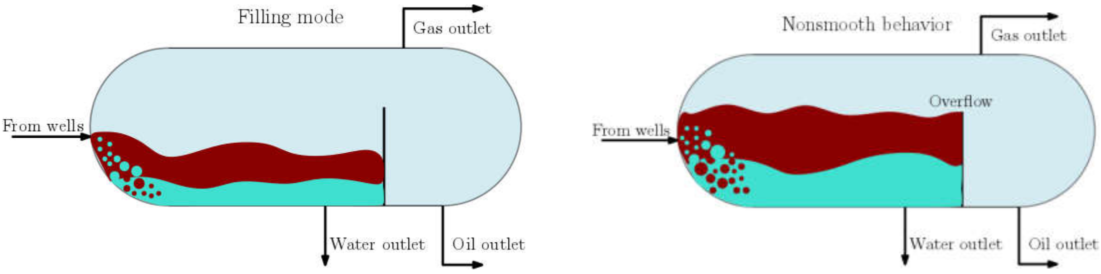
Projects offered by Associated Professor Johannes Jäschke,

JOHANNES.JAESCHKE@NTNU.NO

68 Nonsmooth models for subsea separation systems

Co-Supervisor: Marlene Louise Lund

Many processes contain nonsmooth characteristics in the form of non-differentiable "kinks" in the variables as functions of time. In subsea oil and gas production and handling systems, examples of nonsmooth behavior is related to production start-up and shut-down, flow transitions, flow control and thermodynamic phase changes. The traditional way of handling such behavior is using hybrid models, meaning that a set of models for different regimes is developed with discrete transitions between them. However, this strategy leads to models that are challenging both to formulate and solve. New developments within nonsmooth analysis over the past few years facilitates for easy and automatic solving of nonsmooth models using generalized derivatives. The aim of this project is to formulate a nonsmooth model of a three-phase separator that handles continuous transitions between start-up and production. This includes filling the separator as well as transitions between different phase regimes (see [1]).



Tasks:

- Literature study on nonsmooth analysis
- Study basic separator modeling
- Formulate and implement a separator model using principles form nonsmooth analysis
- Compare with standard modelling methods

Note that this project requires skills within programming (e.g Matlab or another programming language) as well as knowledge about basic mathematics.

[1] Ali M. Sahlodin A., Harry A. J. Watson, and Paul I. Barton, "Nonsmooth model for dynamic simulation of phase changes", Massachusetts Institute of Technology. Published in *AIChE J*, 62: 3334–3351, 2016.

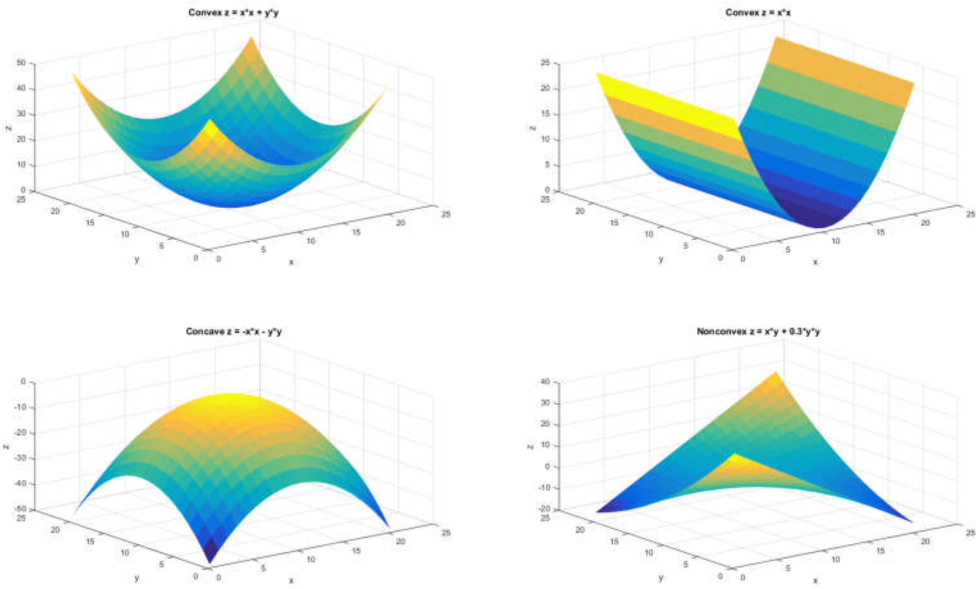
69 PYTHON IMPLEMENTATION FOR PATH-FOLLOWING NLP SENSITIVITY

Co-Supervisor: Eka Suwartadi

Optimization based control has shown its ability to handle chemical processes in safe and economic ways. Model predictive control (MPC) has been widely used in process control industry. MPC relies on robust and reliable numerical optimization algorithms. Due to nonlinearity in dynamical systems which modeled the process, nonlinear MPC is employed instead of the linear one. This requires the use of nonlinear programming (NLP) solvers.

For nonlinear systems with fast time constant, a NLP solver may not be able to find optimal solution in the designated allocated time. This can be detrimental for a nonlinear MPC implementation. To mitigate this problem, NLP sensitivity is deployed to speed up the optimization runtime (see [1,2]). The NLP sensitivity is computed by solving a sequence of quadratic programming (QP) solver. Figure below is an illustration of different types of QP problems.

In this project, student will implement path-following NLP sensitivity algorithms particularly the path-following described in [3]. Student will write Python code and test the implementation on several case examples.



Tasks

- Literature study on NLP sensitivity
- Study numerical optimization algorithms for NLP sensitivity
- Assess efficient quadratic programming (QP) solvers for computing NLP sensitivity
- Write Python code for NLP sensitivity which may include interfaces for existing QP solvers
- Perform testing for the Python implementation for several case examples
- Analyse and foresee the application of NLP sensitivity for nonlinear MPC implementation

Student involved in this work will learn efficient numerical optimization algorithms and get hands-on experience in developing numerical software algorithm. It will be great if the student can contribute to open source numerical optimal control software package such as CasADi.

[1] Diehl, M., Bock, G.H., Schlöder, J.P., Findeisen, R., Nagy, Z., and Allgöwer, F., Real-time optimization and nonlinear model predictive control of process governed by differential-algebraic equations. Journal of Process Control, Volume 12, pp. 577-585, 2002.

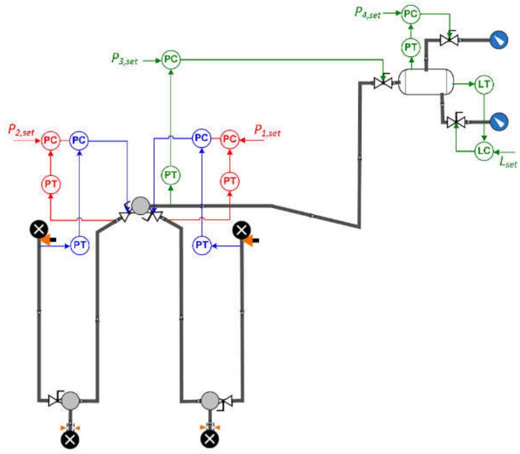
[2] Zavala, V.M., and Biegler, L.T., The advanced-step nmpc controller: optimality, stability, and robustness. Automatica, Volume 45, pp. 80-93, 2009.

[3] Suwartadi, E., Kungurtsev, V., and Jäschke, J., Sensitivity-based economic nmpc with a path-following approach. Processes, 5:1, 2017.

70 Economic model predictive control of oil gathering network

Co-Supervisor: Eka Suwartadi

This project may be done for a group of students since the implementation is not straightforward and requires a good understanding of Kalman Filter and nonlinear model predictive control (NMPC). Idea for this project is from the paper of Codas et. al [1]. Process described in the paper includes a network of two gas-lift oil wells, a common pipeline-riser system and a separator (see figure below). The modeling part is done by using dynamics simulation tool Modelica and real plant model is simulated by using OLGA (multiphase flow simulator). The NMPC implementation is facilitated by CasADi with OpenOPC data communication to OLGA. The whole system implementation is in Python programming language.



Tasks

- First task is to understand the system dynamics. Students will run the existing model and get to know the simulation tools (Modelica, CasADi, and OLGA).
- Literature study on numerical optimization control implementation especially the integration schemes such as single shooting, multiple shooting, and collocation methods.
- Develop economic MPC controller using collocation method instead of multiple shooting which has been implemented in the paper.
- Assess the possibility to speed up the simulation for example using distributed computing platform (multicore CPUs).

[1] Codas, A., Jahanshahi, E., and Foss, B., A two-layer structure for stabilization and optimization of an oil gathering network. In the proceeding of 11th IFAC symposium on dynamics and control of process systems including Biosystems, June 6-8, 2016. NTNU, Trondheim, Norway.

71 MODELLING OF ÅSGARD SUBSEA GAS COMPRESSION STATION FOR CONDITION MONITORING PURPOSES

Co-supervisors: Adriaen Verheyleweghen and Tamal Das

Subsea production and processing of oil and gas can potentially help solve many of the problems associated with platform-based production. By putting the processing equipment on the seabed, we can operate in harsh conditions, far away from the shore, and without need for manned platforms. However, to avoid costly breakdowns that require intervention, it is necessary to have good condition-based maintenance routines. Since we are usually not able to measure the condition of the system directly, we need to estimate it from other plant measurements.

The purpose of this project is to model the Åsgard subsea gas compression station, with the specific goal to use the model for condition monitoring purposes. The student will develop models for estimating the health state of the systems (system diagnostics), but also models which predict the future health degradation of the system if possible (system prognostics). It is advantageous if the student is comfortable with programming in MATLAB and has knowledge of basic optimization.

Expected tasks and learning outcomes:

- Literature study of subsea process systems and condition monitoring
- Modelling of the Åsgard compression station
- Condition monitoring using Kalman filters / moving horizon estimation

FIGURE 1: ARTIST RENDITION OF THE ÅSGARD GAS COMPRESSION STATION. COPYRIGHT: AKER SOLUTIONS

72 Optimal control of a LNG plant

Co-supervisor: Adriaen Verheyleweghen

Efficient energy use is a growing industrial challenge in today's competitive market. This is especially true in large, energy-demanding processes such as refrigeration cycles in the petrochemical industry. Due to the significant power consumption, optimizing the operation of such processes is key. Because many degrees of freedom are available for control, finding the optimal strategy may be non-trivial.

The purpose of this project is to improve an existing model of a LNG liquefaction plant and compare different control strategies, such as self-optimizing control and model predictive control. It is advantageous if the student is comfortable with programming in MATLAB and has knowledge of basic optimization.

Expected tasks and learning outcomes:

- Literature study of refrigeration plants and optimal control strategies
- Modelling of a LNG plant
- Comparison of several control strategies

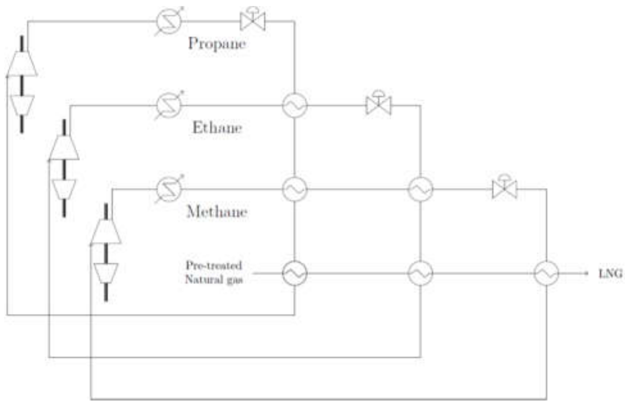
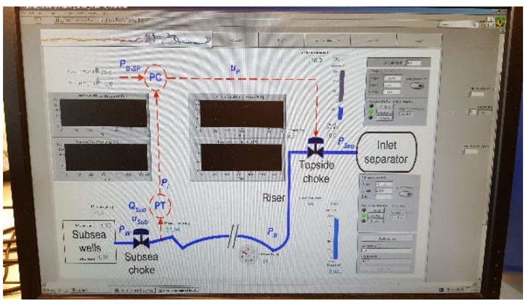


FIGURE 2: CASCADE REFRIGERATION SYSTEM FOR NATURAL GAS LIQUEFACTION

73 ANTI-SLUG LAB

Co-supervisor: Tamal Das and Sigurd Skogestad

In multiphase flows, gas and liquid phases coexist to form several di erent flow regimes. Commonly known flow regimes include stratified flow, bubbly flow etc. The flow regimes adopted by fluids in a pipe are largely dependent on the gas flow rate, the liquid flow rate and the orientation of the pipe. In the vertical orientation of the pipe with the fluids flowing upwards, it is sometimes challenging to ensure a uniform flow, especially in a flow regime called slug flow. In slug flow, there is a pressure built up at the bottom of the vertical pipe near the inlet because the vertical pipe is fully filled with a liquid column. Eventually, the gas pressure rises higher than the hydrostatic pressure in the column causing a blowout of the liquid column. This causes alternating periods of no flow and blow outs. Hence, from a process engineering perspective slug flow is undesirable. A common approach to avoid slugging is to decrease the inlet flow by choking down the inlet valve. However, this approach leads to reduced throughput. Automatic control of the bottom pressure (or similar approaches) in order to avoid slugging is known as anti-slug control. In this project, the student will have access to the anti-slug lab (with a computer running LABVIEW with manual/automatic control, where the whole process can be visualized), where the student will get familiarized to the phenomenon of slugging and how to control it using the available choke valves in order to ensure uniform flow.



To systematically design an anti-slug controller, one needs a model, which has already been developed in the group [1]. This model will be the basis for some analysis. Once the basic understanding of the model based controller design is in place, the student will develop under-standing of state estimation to estimate the unmeasured variables in the model presented in [1] using the available measurements, such as pressures. Further, state estimation principles can be used for flow estimation and slug detection, which can be verified against the data from LABVIEW. The estimated variables could be used in the control design.

State estimation is usually dependent on the measurements. What if the measurements are slightly wrong because the sensor is malfunctioning, i.e. the pressures measured have a bias. Accurate information of the unmeasured variables can still be retrieved using gross error detection [2].

Finally, all state estimation methods rely on tuning of the estimators (such as Kalman filters). The tuning usually refers to determining process noise covariance matrix and the measurement noise covariance matrix. These matrices are hard to get in real applications. Hence, a method called auto-covariance least squares [3] will be used to see how much it impacts the estimation performance. The student can direct the project to his/her liking.

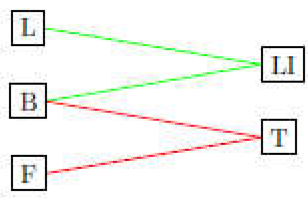
References

[1] E. Jahanshahi, "Control solutions for multiphase flow: Linear and nonlinear approaches to anti-slug control," 2013.
[2] B. Nicholson, R. L´opez-Negrete, and L. T. Biegler, "On-line state estimation of nonlinear dynamic systems with gross errors," Computers & Chemical Engineering, vol. 70, pp. 149–159, 2014.
[3] B. J. Odelson, A. Lutz, and J. B. Rawlings, "The autocovariance least-squares method for estimating covariances: application to model-based control of chemical reactors," IEEE transactions on control systems technology, vol. 14, no. 3, pp. 532–540, 2006.

74 TEMPERATURE AND LIGHT INTENSITY CONTROL

Co-supervisor: Tamal Das

Learning process control on real applications is exciting. Hence, we o er a project to learn from experimenting with process control strategies on a small equipment known as PSE-5. The underlying process is a MIMO system (Multiple input multiple output), with three inputs and two outputs. The inputs are LED (L), BULB (B) and FAN (F) and the outputs are LIGHT-INTENSITY (LI) and TEMPERATURE (T). L and B a ect the LI with a zero order dynamics, whereas B and F a ect the T with a first order dynamics.



The system can be easily plugged into a computer and visualized in SIMULINK, from where one could easily do manual or automatic control. The project will start with system identification using MATLAB system identification toolbox. Using the identified model, the control will be designed. Ideally speaking, T control using PID is very easy if using only B. However, a faster control can be achieved with using both B and F (MIMO control). On the other hand F could be used as a disturbance. Similarly, for the LI control, both B and L can be used. If one wants to control the LI without impacting the T, L is the best choice as the manipulated variable. But, L has a limit to which it can a ect the LI. For higher LI, one needs to use B, but B a ects the T. Hence, to do a combined control of T and LI, one needs to use all the inputs in an optimal way, which could lead to some optimal control strategies, such as, but not limited to, linear quadratic regulator.

Next, some state estimation principles will be used to estimate some variables considered un-measured (even though they are measured), such as bulb power or fan speed. This will be done to verify how accurate the estimation works against the measured values for the same variables. State estimation is usually dependent on the measurements. What if the measurements are slightly wrong because the sensor is malfunctioning, i.e. the temperature measured has a bias. Accurate information of the unmeasured variables can still be retrieved using gross error detection [1].

Finally, all state estimation methods rely on tuning of the estimators (such as Kalman filters). The tuning usually refers to determining process noise covariance matrix and the measurement noise covariance matrix. These matrices are hard to get in real applications. Hence, a method called auto-covariance least squares [2] will be used to see how much it impacts the estimation performance.

The student can direct the project to his/her liking.

References

[1] B. Nicholson, R. L´opez-Negrete, and L. T. Biegler, “On-line state estimation of nonlinear dynamic systems with gross errors,” Computers & Chemical Engineering, vol. 70, pp. 149–159, 2014.
[2] B. J. Odelson, A. Lutz, and J. B. Rawlings, “The autocovariance least-squares method for estimating covariances: application to model-based control of chemical reactors,” IEEE transactions on control systems technology, vol. 14, no. 3, pp. 532–540, 2006.

75 FLOW ESTIMATION

Co-supervisor: Tamal Das

Virtual flow metering is estimation of flow using easily available measurements, such as pressure and temperature. This field of research is very sought after because physical flow meters, especially for multiphase flows, are very expensive and tend to be inaccurate. In subsea oil and gas industry, accurate measurement/estimation of phase flows are important because the revenues for the companies sharing the same production infrastructure rely on it. This project will rely on state estimation techniques, such as Kalman filtering, Extended Kalman filtering, Moving horizon estimation to name a few. Based on which techniques are used, the student can have exposure to Kalman based filtering methods or optimization based moving horizon estimation. Moving horizon estimation will involve dynamic optimization using CasADi, an algorithmic di erentiation tool. For state or parameter estimation, one needs a model. In the literature, there exist several models. These models fit into di erent classes of flow estimation: static or dynamic estimation, two phase model or three phase model, no slip between gas-liquid or slip between gas-liquid (Drift flux model), unilateral wells (without tie-ins) or multilateral wells (with tie-ins), flow regime dependent models or flow regime independent models.

The project will commence with a quick literature survey on flow estimation oriented mod-els. Simultaneously, the student will deepen understanding in state estimation techniques and casADi (if dynamic optimization based estimators are chosen). Based on this, flow estimation will be tested in MATLAB/Modelica (Dymola/OpenModelica) using relevant models found in the literature. These models will be the basis for some further analysis. The next step would be to test the flow estimation methods against the industry approved dynamic multiphase flow simulator OLGA. It is possible to connect OLGA to MATLAB/Modelica using an OPC server such as Matrikon.

State estimation is usually dependent on the measurements. What if the measurements are slightly wrong be-cause the sensor is malfunctioning, i.e. the pressures measured have a bias. Accurate information of the unmeasured variables can still be retrieved using gross error detection [1]. This could be a potential direction for developing an estimator robust to gross error.

Finally, all state estimation methods rely on tuning of the estimators (such as Kalman filters). The tuning usually refers to determining process noise covariance matrix and the measurement noise covariance matrix. These matrices are hard to get in real applications. Hence, a method called auto-covariance least squares [2] will be used to see how much it impacts the estimation performance.

The student will have the flexibility to direct the project to his/her own liking.

References

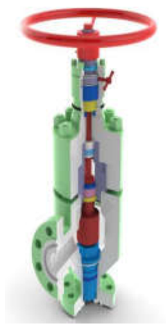
[1] B. Nicholson, R. L´opez-Negrete, and L. T. Biegler, "On-line state estimation of nonlinear dynamic systems with gross errors," Computers & Chemical Engineering, vol. 70, pp. 149–159, 2014.
[2] B. J. Odelson, A. Lutz, and J. B. Rawlings, "The autocovariance least-squares method for estimating covariances: application to model-based control of chemical reactors," IEEE transactions on control systems technology, vol. 14, no. 3, pp. 532–540, 2006.

76 CONDITION MONITORING OF CHOKE VALVES

Co-supervisor: Adriaen Verheylewegen and Tamal Das

In subsea processing of oil and gas, equipment redundancy is crucial to ensure no loss in production. One of the drawbacks of having equipment on the seabed is that they can not be maintained all the time. Any major or minor changes to the equipment or retrieval for maintenance needs to be planned much in advance. Hence, it is important to monitor the condition of the critical equipments that tend to breakdown frequently. For a quick overview on the subsea condition monitoring systems, refer [1].

Choke valves can break down due to many failure mechanisms. Sand erosion and corrosion are a few of those. In this project, we will focus on determining the condition of choke valves using commonly available measurements around the choke valves, such as di erential pressure between inlet and outlet. The condition can be estimated using a mathematical model, some measurements and state/parameter estimation techniques. For example, the pressure, temperature and flow rate measurements can be used to estimate the current flow coe cient (C_v) of a choke valve. This C_v can be compared to the reference C_v (from vendors); if it is higher than the reference, it is likely that the choke valve has a damage. If there are major changes in current C_v, it indicates accelerated damage [2]. Choke flow models can be found in [3] and erosion models can be found in [4].



The project will commence with a quick literature survey to identify the relevant models. Then, the models will be used to predict the condition of the choke valves. The overall choke valve behavior is a gross indicator of worsening condition, which could be a ected due to several failure mechanisms. We intend to focus on erosion and corrosion. The result of this project will be a system that can take the necessary measurements and provide some variables that are key indicators of health of choke valves, such as C_V (diagnostic) and how these variables will develop in future (prognostic).

State estimation methods such as Kalman filters will be used to fuse the information from the models and the measurements to estimate the condition of the choke valve. The tuning of filters are hard in real applications, which usually means determining process noise covariance matrix and the measurement noise covariance matrix. Hence, a method called auto-covariance least squares [5] will be explored.

The student can direct the project to his/her liking.

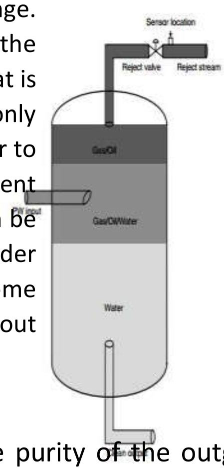
References

[1] L. P. Chze, C. W. Liam et al., "Optimising data processing for subsea system surveillance through subsea condition monitoring," in O shore Technology Conference Asia. O shore Technology Con-ference, 2016.
[2] C. Soosaipillai, P. K. Roald, D. Alfstad, T. Aas, G. Smith, J.-Y. Bressand et al., "Condition perfor-mance monitoring for subsea: Experience and value documentation from the gjoa field," in O shore Technology Conference. O shore Technology Conference, 2013.
[3] R. Sch¨uller, T. Solbakken, S. Selmer-Olsen et al., "Evaluation of multiphase flow rate models for chokes under subcritical oil/gas/water flow conditions," SPE production & facilities, vol. 18, no. 03, pp. 170–181, 2003.
[4] R. Paggiaro, J. D. Friedemann, E. Gharaibah, Y. Zhang et al., "Prediction of sand erosion in choke valves-cfd model development and validation against experiment," in OTC Brasil. O shore Tech-nology Conference, 2013.
[5] B. J. Odelson, A. Lutz, and J. B. Rawlings, "The autocovariance least-squares method for estimating covariances: application to model-based control of chemical reactors," IEEE transactions on control systems technology, vol. 14, no. 3, pp. 532–540, 2006.

77 COMPACT FLOTATION UNIT MODEL

Co-supervisor: Tamal Das

In subsea oil and gas industry, produced water treatment is a significant chal-lenge. Produced water (PW) is the water produced along with oil from the reservoir. After the bulk separation of oil and water, the separated water still con-tains amount of oil that is neither suitable for reinjection into the reservoir nor for rejection into sea. Commonly used equipment in the industry to reduce the oil-in-water content in produced water to ppm levels are hydrocyclones (HC) and Compact flotation units (CFU) [Figure 1]. Recent advances in CFUs for produced water treatment and their functional description can be found in [2]. In this project, we want to develop a steady state model of a CFU in order to calculate the separation e ciency under given PW flow rate and gas flow rate. Some mechanisms for CFU modeling can be found in [3]. Additional information about operation and optimization of PW in CFU can be found in [4].



The next step would be to develop a dynamic model that can provide the purity of the outgoing streams based on the inlet and operating conditions. This model will be used for controlling the process or estimating key variables of interest using available measurements. The student will, therefore, deepen understanding of state and parameter estimation techniques, such as Kalman Filters.

Key inspiration for the modeling work can be found in two chapters, namely Equipment for Gas-Liquid Operations (Chapter 6) and Gas Absorption (Chapter 8) in [5] and example 18.4-1 in [6]. Further, gas flotation theory will be explored to develop the model.

The student can direct the project to his/her liking.

References

[1] B. K. Arvoh, S. Asdahl, K. Rabe, R. Ergon, and M. Halstensen, “Online estimation of reject gas and liquid flow rates in compact flotation units for produced water treatment,” Flow Measurement and Instrumentation, vol. 24, pp. 63–70, 2012.
[2] M. Bhatnagar, C. J. Sverdrup et al., “Advances in compact flotation units (cfus) for produced water treatment.” in O shore Technology Conference-Asia. O shore Technology Conference, 2014.
[3] M. Maelum, K. Rabe et al., “Improving oil separation from produced water using new compact flota-tion unit design,” in SPE Production and Operations Symposium. Society of Petroleum Engineers, 2015.
[4] S. Asdahl, K. Rabe et al., “Real-time automatic operation and optimization of produced-water treat-ment,” in SPE Middle East Intelligent Energy Conference and Exhibition. Society of Petroleum Engineers, 2013.
[5] R. E. Treybal, “Mass transfer operations,” New York, 1980.
[6] R. B. Bird, W. E. Stewart, and E. N. Lightfoot, Transport phenomena. John Wiley & Sons, 2007.

PROJECTS OFFERED BY PROFESSOR SIGURD SKOGESTAD, SKOGE@NTNU.NO

78 PROCESS CONTROL CASE STUDY AT PERSTORP

Supervisors: Krister Forsman and Sigurd Skogestad

Krister Forsman is Professor II at NTNU and has given guest lectures in the process control course about industrial control strategies. He leads the control group at Perstorp, which is a Swedish chemical company with many plants all over the world and many intersting control problems. To keep the application current and of interest to Perstorp the specific application will be decided later. The work will generally involve the following (mostly using Matlab):

1. Derive a simple process model (Simulink/Matlab)

2. Match to current operation data

3. Propose an improved control strategy. This will often involve suggestions for moving the throughput manipulator and introducing cascades or simple model-based strategies.

Typically, the project may deal with the modelling and matching with data, and the master thesis will focus on the control part.

79 PROCESS CONTROL CASE STUDY AT NORSKE SKOG

Co-supervisor at Norske Skog, Skogn: Andreas Volden

There are several possible case studies, most related to effective use of enegy. One of them is the steam system and another is the heat recovery from combustion. More details will be published on the home page of Sigurd Skogestad soon (see under project students).

The project will focus on modelling and comparing with data from the real plant and the master thesis will focus on control.

80 Modeling and simulation of an inclined pipe separator

The task of the candidate will be to develop a mathematical model (dynamic / steady state) of an inclined pipe separation process with application to the oil and gas industry and potential subsea application. A pipe separator is a separation device working on the principle of separation by density differences and gravitational forces and is by principle related to gravity separators.

Specific tasks include:

- Literature review of potentially existing pipe separator models as well as inclined pipe separators with industrial applications that have already been established
- Modeling of the major dynamic / steady state principles by means of first principles / physical phenomena
- Development of a simulation model to test and verify the mathematical model in a software like Matlab/Simulink and/or Modelica
- Writing a project report about the conducted work including and describing the above-mentioned points

The project will be conducted during the fall semester 2017 at the Department of Chemical Engineering under the supervision of Prof. Sigurd Skogestad and Dr. Christoph J. Backi.
The project is part of SUBPRO (SFI Center for Subsea production and processing).

81 Modeling and simulation of a gravity separation device for oil and gas applications

The task of the candidate will be to improve and further develop the mathematical model of a gravity separator introduced by C.J. Backi. A gravity separator is a device based upon the principles of separation by density differences and gravitational forces. It is widely used in the oil and gas industry and serves as a bulk separation device.

Specific tasks include:

- Literature review of existing gravity separator models and related principles (such as particle balances)
- Working and understanding the model developed by C.J. Backi and afterwards incorporating new phenomena into the model. These can include coalescence and/or breakage of droplets as well as a dense-packed layer interface.
- Extend the simulation model to test and verify the mathematical improvements in a software like Matlab/Simulink and/or Modelica
- Writing a project report about the conducted work including and describing the above-mentioned points

The project will be conducted during the fall semester 2017 at the Department of Chemical Engineering under the supervision of Prof. Sigurd Skogestad and Dr. Christoph J. Backi.
The project is part of SUBPRO (SFI Center for Subsea production and processing).

82 ADAPTIVE ANTI-SLUG CONTROL

The task of the candidate will be to improve and further develop the mathematical model of a gravity separator introduced by C.J. Backi. A gravity separator is a device based upon the principles of separation by density differences and gravitational forces. It is widely used in the oil and gas industry and serves as a bulk separation device.

Specific tasks include:

• Literature review of existing anti-slug control algorithms, including adaptive kinds

• Working and understanding the anti-slug model developed by E. Jahanshahi

• Test the developed control structures in Matlab/Simulink and afterwards in the anti-slug lab at the Department of Chemical Engineering

• Writing a project report about the conducted work including and describing the above-mentioned points

The project will be conducted during the fall semester 2017 at the Department of Chemical Engineering under the supervision of Prof. Sigurd Skogestad and Dr. Christoph J. Backi.

The project is part of SUBPRO (SFI Center for Subsea production and processing).

Project: Simple pump characteristic models based upon analytical expressions

The task of the candidate will be to investigate pump curve characteristics with respect to e.g. flow, head and rotational speed and find simple, analytical expressions for these pump curves. Further variables can include power consumption, efficiency, net positive suction head, etc.
Specific tasks include:

• • Literature review of pumps and potential existing work on simple pump characteristics modeling

• • Comparison of the simple analytical pump characteristics with existing lookup-table-based characteristics in simulation environments such as Matlab/Simulink with respect to performance. HYSYS or other environments could also be used.

• • Writing a project report about the conducted work including and describing the above-mentioned points

The project will be conducted during the fall semester 2017 at the Department of Chemical Engineering under the supervision of Prof. Sigurd Skogestad and Dr. Christoph J. Backi. The project is part of SUBPRO (SFI Center for Subsea production and processing).

83 SIMPLE PUMP CHARACTERISTIC MODELS BASED UPON ANALYTICAL EXPRESSIONS

The task of the candidate will be to investigate pump curve characteristics with respect to e.g. flow, head and rotational speed and find simple, analytical expressions for these pump curves. Further variables can include power consumption, efficiency, net positive suction head, etc.

Specific tasks include:

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The project will be conducted during the fall semester 2017 at the Department of Chemical Engineering under the supervision of Prof. Sigurd Skogestad and Dr. Christoph J. Backi. The project is part of SUBPRO (SFI Center for Subsea production and processing).

84 OPTIMIZATION OF THE SYNTHESIS-GAS LOOP AS EXAMPLE FOR INTEGRATED PROCESSES.

Supervisor: Julian Straus and Sigurd Skogestad

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.

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 replace the sub-model itself with a simplified (surrogate) model. The surrogate models are then combined and optimization can be performed [1].

The definition of surrogate models and the sampling using the detailed model is however complicated partly due to the flowsheet topology and partly due to many connectivity variables.

The task of the project is set within the Ph.D. project of Julian Straus on optimization of integrated processes.

Depending on the process until August, several possibilities may arise about the exact nature of the project. Prospective students are encouraged to bring in own ideas. Generally, the project will involve extensive MATLAB modelling as well as MATLAB-HYSYS interaction. The student is required to have good knowledge in MATLAB.

If questions arise and/or you are interested in the project, feel free to contact me (julian.straus@ntnu.no, or pass by in room K4-239).

[1] J.Straus, S. Skogestad, *Computer Aided Chemical Engineering* **2016**, 38, 289-294.

85 MODELLING A SUBSEA PRODUCTION NETWORK

Co-supervisor: Dinesh Krishnamoorthy

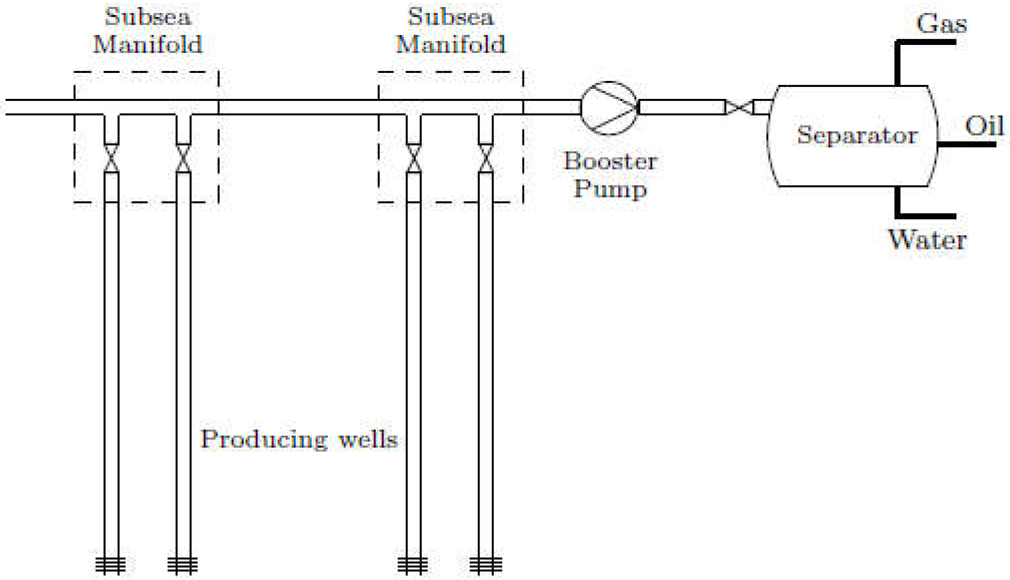
Subsea production systems consists of many interconnected wells and processes such as compressors and booster pumps. Models that represents the production network are crucial for Daily Production optimization. The main task of this project is to develop a subsea production network with different manifolds that are interconnected and produce to a common riser manifold equipped with a subsea boosting station.

Possible tasks of this project are:

- Use gas lifted well model as building blocks to model a large subsea production network (preferably that matches the Shell Draugen case)
- Model a subsea multiphase booster pump
- Implement simple pressure and flow controllers (regulatory control)

The project requires basic knowledge of modelling and control. Models should ideally be developed in MATLAB.

This project is part of SUBPRO. For any questions and/or you are interested in this project, feel free to contact Sigurd Skogestad or Dinesh Krishnamoorthy (dinesh.krishnamoorthy@ntnu.no).



86 ADAPTIVE MPC OF A SUBSEA SYSTEM

Co-supervisor: Dinesh Krishnamoorthy

Subsea production systems consists of many interconnected wells and processes such as compressors and booster pumps. Models used for production optimization are subject to uncertainty due to lack of knowledge or model simplification. One way to handle unknown disturbances or structural uncertainty is to use an adaptive controller. In this project we propose to use an adaptive linear MPC to adapt the models online using measurements.

- The main aim of this project is to develop an Adaptive MPC scheme

- And test the developed controller using a gas lifted well simulator

The project requires basic knowledge of control and estimation. Models of gas lifted well network are available and the focus of the project is on developing adaptive MPC (preferably in MATLAB or SEPTIC).

This project is part of SUBPRO. For any questions or if you are interested in this project, feel free to contact Sigurd Skogestad or Dinesh Krishnamoorthy (dinesh.krishnamoorthy@ntnu.no).

87 Extremum seeking control of a subsea production network

Co-supervisor: Dinesh Krishnamoorthy

Subsea production systems consists of many interconnected wells and processes such as compressors and booster pumps. Models used for production optimization are subject to model structural uncertainty due to lack of knowledge or model simplification. One way to handle unknown disturbances or structural uncertainty is to use a model free method. Extremum seeking control is one such model free optimization method that can be used to optimize a production network. Extremum seeking control uses the measurements to estimate the local gradient and converges to the optimum.

- The main aim of this project is to develop extremum seeking controllers to optimize production from a gas lifted well network.
- Additionally, extremum seeking control can be combined with self-optimizing control to further improve the performance.

The project requires basic knowledge of control and estimation. Models of gas lifted well network are available and the focus of the project is on extremum seeking control and self-optimizing control. The controllers can be developed in MATLAB or SEPTIC.

This project is part of SUBPRO. For any questions or if you are interested in this project, feel free to contact Sigurd Skogestad or Dinesh Krishnamoorthy (dinesh.krishnamoorthy@ntnu.no).

Biorefinery and Fiber Technology

Projects offered by Associate Professor Størker Moe storker.moe@ntnu.no s

88 Organosolv pretreatment of biomass for hydrolysis

Organosolv pretreatment is an interesting process for biorefinery applications, since it yields a less modified lignin stream than other pretreatment processes do. This enables utilization of the lignin fraction of biomass for more value-added applications like bio-based phenolic chemicals, resins etc.

The aim of the project will be to investigate organosolv pretreatment in our newly installed autoclave reactor system, tuning the system and providing basic data for further investigations of the organosolv pretreatment process

Supervisor: Størker Moe

89 Establishment of a Hysys model for the chitosan production process

Chitosan is a biopolymer manufactured from crustacean shells. The current production process involves the use of substantial amounts of mineral acid and sodium hydroxide, and the waste streams are not easily utilized. However, attempts[1] have been made at using proteases instead of NaOH for the deproteinization of the raw material, and this may enable exploitation of the waste stream from the deproteinization stage for manufacture of protein hydrolyzates.

The project will include a combination of process modeling in Aspen Hysys, and literature studies to investigate the feasibility of utilizing the deproteinization stage waste water for production of protein hydrolysates as a byproduct.

Supervisor: Størker Moe
Co-supervisor: Magne Hillestad

90 Extension of a Hysys biorefinery model

A model for a biorefinery producing ethanol and furfural from has been developed[2] in Hysys. The model still needs further development, particularly in the fermentation process chapter, and in the waste recovery/energy production process chapter.

Supervisor: Størker Moe
Co-supervisor: Magne Hillestad

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1 Younes, I. et al. (2012): "Chitin and chitosan preparation from shrimp shells using optimized enzymatic deproteinization", *Process Biochemistry* **47**(12), 2032–2039, http://dx.doi.org/10.1016/j.procbio.2012.07.017

2 Strømsnes, L.M. (2016): "Process Modeling of a Biorefinery for Integrated Production of Ethanol and Furfural in HYSYS", MSc thesis, NTNU.

91 Determining liquid-vapor equilibria for the modeling of an alcohol-based process for a renewable, environmental-friendly wood-based material

Kebony is a modified wood product made by impregnating wood with furfuryl alcohol (furfurol) and subsequently polymerizing the furfurol in situ. The material is made completely from renewable raw materials, free from heavy metals and environmentally malign components and very stable towards degradation. It has therefore captured a market among customers where environmental-friendly stability towards degradation is a priority. The company now wants to develop a process using an alcohol-based impregnation solution, to produce a product suitable also for marine applications.

An alcohol-based process will require solvent recovery and a new production process. The project has recently been awarded a grant from Oslofjordfondet for the development of the new process, and one important issue is a successful modeling of the solvent recovery system. The process model will require non-steady state (dynamic) modeling of a batch process, with little available reliable liquid-vapor equilibrium data. It's therefore important to acquire experimental data for use in the model calculations.

The project will entail experimental determination of liquid-vapor equilibria in various alcohol/water/furfurol mixtures, and design of a simple model of a proposed recovery process. The project is a part of the Oslofjord Regional Research Fund financed R&D project 269707 "Alcohol based process for wood furfurylation".

The project may be continued and expanded in an MSc thesis project.

Projects offered by Professor Øyvind W. Gregersen oyvind.w.gregersen@ntnu.no

92 Study the effect of mimic enzyme in PVA/Nano cellulose films on CO_2 permeation and selectivity of membranes

Background:

The global emission of carbon dioxide has risen for many decades, and in recent years, there has been an increasing awareness of the impact of greenhouse gas emissions with scientific models substantiating the claims. Carbon Capture and Storage is considered as one option for reducing global emission. Currently, Use of polymeric membranes for CO_2 capture is an emerging field of research. A main objective of the membrane development work is to achieve an improved combination of selectivity and permeability of the membrane.

New membrane technologies such as facilitated transport (FT) and fixed-site carrier membranes are of interest to increase both selectivity and permeability. Facilitated transport selectivity enhances the permeability of a targeted gas by incorporating a carrier in the membrane. Polyvinyl alcohol (PVA) membranes have received significant attention in this field. Water can act as a carrier for CO_2 in such membranes. Additionally, a mimic enzyme can also be added as a carrier in PVA membranes. This raises the question of how to gain and maintain a carrier such as water and mimic enzyme in the membranes. Cellulose nanofibrils (CNF) and cellulose nanocrystals (CNC) have received much attention in the past decades as a new reinforcing material in polymer composites. They are used as an excellent filler particle in FT membranes.

The Project:

This work involves the casting and characterization of different types of polymeric membranes used for biogas upgradation. Addition of Nano cellulose is supposed to increase the performance of the water swollen membrane. The presence of nanocellulose in polymeric membranes has been studied in detail [2]. The possible effects of Nano cellulose would be increased degree of swelling, increased swelling rate and to increase the molecular porosity. These mechanisms need to be investigated in detail by using characterization techniques.

Further Zn base mimic enzyme will be added in these composite membranes in order to speed up the dissociation of the dissolved CO_2.

In this work, facilitated transport membranes will be synthesized using PVA, nanocellulose and mimc enzyme. Addition of mimic enzyme is a relatively new idea. Recently, Muhammad Saeed, a PhD at MEMFO group, did work in this field. His work showed promising results for selectivity and permeability of CO_2 after addition of mimic enzyme [3]. Mimic enzyme is an artificially made chemical compound that resembles naturally existing carboxylase enzyme used by living organisms to capture CO2. Mimic enzyme used for his research work was synthesized in MEMFO lab at NTNU and was characterized with the help of H^1NMR and ESIMS to validate its existence.

Keeping this background, the aim of this work will be structural characterization of PVA- Nano cellulose and mimic enzyme based membranes for biogas separation. This composite membrane will consist of a thin dense polyvinyl alcohol (PVA) selective layer containing a low molecular weight mimic enzyme and a polysulfone (PSF) ultrafiltration porous support. In this work, the effect of varying mimic enzyme composition will be studied. Dip coating will be used to cast membranes on a polysulfon support. These membranes will be tested in the high pressure membrane rig under humidified conditions [4].

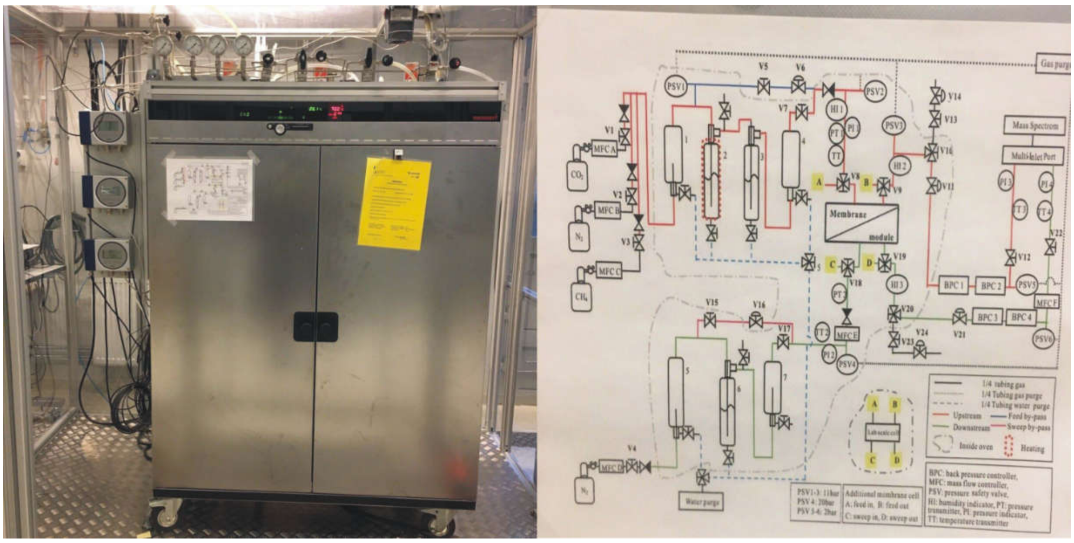

Fig 1. High pressure membrane rig.

Experimental Work:

These composite membranes will be tested for their performance (permeability and selectivity) at different operating pressure conditions varying from 5 bar to 20 bar, keeping constant feed composition and flowrates. It is required to characterize membranes surface and cross section using SEM before and after use to see how high pressure and humidified conditions affect the membrane morphology.

Supervisor: Øyvind Weiby Gregersen (oyvind.w.gregersen@ntnu.no), Co supervisor: Zaib Jahan (zaib.jahan@ntnu.no)

References:

1. Lloyd M. Robeson, ”The upper bound revisited”. Journal of Membrane Science, 2008. 320: p. 390-400.
2. Henrik Riis, “Development of structural characterization methods for polyvinyl alcohol (PVA)/Nanocellulose composite membranes”. Department of Chemical Engineering, 2016. Norwegian University of Science and Technology.
3. Muhammad Saeed and Liyuan Deng, “Post-combustion CO2 membrane absorption promoted by mimic enzyme”. Journal of Membrane Science, 2016. 499: p. 36-46.
4. Muhammad Saeed and Liyuan Deng, “CO2 facilitated transport membrane promoted by mimic enzyme”. Journal of Membrane Science, 2015. 494: p. 196-204.