

# TKP4550/TKP451 PROSESS-SYSTEMTEKNIKK (Process Systems Engineering)

**Coordinator: Professor Sigurd Skogestad**

**Project proposal: Professor Sigurd Skogestad: [sigurd.skogestad@chemeng.ntnu.no](mailto:sigurd.skogestad@chemeng.ntnu.no)**

## **1: Optimal operation of parallel systems**

In order to use the available energy resources optimally, it is often necessary to recover as much heat as possible from a process. This can often be done using a self-optimizing control structure. The idea of self-optimizing control is to achieve near-optimal control by keeping certain variables or variable combinations constant. For heat exchanger networks with parallel branches, we have developed a simple polynomial variable combination which we are considering for a patent application. The objective for this work is to further study the method by considering specific applications, for example, a process stream which is heated using the heat from different batch processes.

The main task is to set up a model of the process and to implement the polynomial variable combinations. Matlab and Simulink will be used for simulations

**Co-supervisor: Jophannes Jäschke (postdoc)**

## **2: Modelling and control of a Bio diesel plant**

The task is to develop a model for a Bio diesel plant. The project tasks are 1. a literature review on bio diesel, 2. setting up a steady state model 3. Simulation and optimization of the model 4. Design of a control structure.

**Co-supervisor: Jophannes Jäschke (postdoc)**

## **3: Modelling, control and optimization of multiphase Heat exchangers**

This project is motivated by our difficulties in optimizing LNG (liquefied natural gas) processes, but also other (simpler) processes may be considered. Optimizing LNG processes is very difficult due to phase change in the heat exchangers and due to mixed refrigerants, which have very non-linear behaviour. Moreover, tight integration and small temperature differences between the streams make the problem numerically challenging.

However, in order to find good control structures, it is necessary to design a model such that it can be used in an optimization software.

The task for this project is to model and optimize a multistream/multiphase heat exchanger using e.g. a new disjunct programming approach, as is described in Kamath et al.  
<http://onlinelibrary.wiley.com/doi/10.1002/aic.12565/pdf>

This project requires good math skills and the ability to work independently. Although the project is not an easy one, it can be a very rewarding one, because the first task is to reproduce the results in the paper by Kamath et al. The main focus of the project is on the modeling and simulation. In a follow-up master project, the focus will be on using the model for control structure design or extending it to mixed refrigerants.

The simulations will be done in the modeling languagesAMPL or GAMS.

**Co-supervisor: Jophannes Jäschke (postdoc)**

## **4: Control strategies for divided wall (Petlyuk) columns**

Divided wall columns offer large potential savings in energy and capital costs, but control remains a difficult issue. The task is to test by dynamic simulations alternative control structures. The objective is to find a simple and robust structure, for example, based on a combination of temperature loops and outer composition loops. The project will start by testing some proposals recently made in our

group (Dwivedi, Halvorsen, Skogestad) and comparing with other suggestions (e.g., Luyben). For simulation of the column one may use Matlab or Unisim/Hysys.

### **5: Control structure design for a sequence of distillation columns**

A good control structure has to optimally adapt to changing product prices in order to run the process as profitably as possible. The task of this project is to design control structures for a sequence of distillation columns.

The project consists of modelling the Distillation columns in a modelling language like ampl and to use the sensitivity features of the software IPOPT to extract information needed to design a good control structure. This is a follow-up work of a well-going existing project and requires good skills with programming languages e.g. matlab/ampl.

### **6: Temperature control for exothermic CSTR**

Controlling the temperature in an exothermic chemical reactor poses a challenge, since the process itself is both non-linear and unstable. In many cases the process has a time delay, because the cooling is effectuated by a cooling water flow, the influence of which takes some time to reach the reactor solution. This is the case regardless of whether the heat exchanger is placed inside the reactor, or in an exterior circulation loop the reactor. These three factors (non-linearity, instability, delay) alone make this control problem quite a challenging one. In addition we have process variations that require the control to be robust. We study continuous stirred reactors. Within the Perstorp group there are several reactors of this type.

A project plan may look as follows. The scope can be reduced if there is not enough time available:

- Verify the mass and heat balances, and linearize this model around a generic equilibrium.
- Investigate which simple PID controller tuning methods that are available for this type of linear processes. If there are none, then suggest one.
- Match the parameters in the suggested tuning method with the physical parameters of the process.
- Quantify fundamental limitations on control performance.
- Can normal operations data be used to estimate the kinetics parameters  $k_0$  and  $E_a$ ?
- Will a non-linear controller structure significantly improve achievable control performance?

For more information see: <http://www.nt.ntnu.no/users/skoge/diplom/prosjekt12/>

**Co-supervisor: Krister Forsman, Perstorp AB**

### **7: Evaluation of SIMC PID-rule.**

We have recently tested the optimality of the SIMC PI-rule and found it to be surprisingly good (see reference below). Actually, this work was done as part of a project by Chriss Grimholt in 2010. We now would like to extend the work to PID control, that is, we want to compare the SIMC PID-rule and compare it with the optimal PID-controller.

Tasks

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

**Cosupervisor: Chriss Grimholt (PhD student)**

### **8: "Optimal PI-Control and Verification of the SIMC Tuning Rule".**

**Proceedings *IFAC conference on Advances in PID control (PID'12)*, Brescia, Italy, 28-30 March 2012.**

<http://www.nt.ntnu.no/users/skoge/publications/2012/grimholt-pi/>

**Chriss Grimholt and Sigurd Skogestad.**

**9: Performance and Robustness of Smith Predictor Controller.**

We want to test the performance and robustness of a Smith Predictor controller for processes with large time delays, by comparing it with PI and PID control. The performance is obviously better if the time delay is known, but it is claimed that it performs poorly if the time delay varies. For example, how does the Smith Predictor perform if the time delay is reduced to zero, or if the time delay is doubled (which are changes that are easily handled using a PI controller)?

**10: Finding the active constraints regions**

The idea of self optimizing control is to achieve a near optimal operation by keeping some "magic" controlled variables constant using the available degrees of freedom. For a given optimal nominal point all the constraints that are active are perfect candidates for self optimizing controlled variables so ideally we would like to keep them constant at their constraints but the major problem is that the set of the active constraints may change when the process is disturbed. The main idea of this project is to develop an online algorithm that will be able to predict the changes in the active constraint set as a function of disturbances. As a case study any Matlab or Hysys/Unisim process model can be used.

**Cosupervisor: Minasidis Vladimirov (PhD student)**

**11: Student projects regarding anti-slug control**

**Slug 1- Simplified model for expansion driven (density-wave) instability**

There are two types of instability occurring in gas-lifted oil wells, namely "casing-heading" and "density-wave", which both result in production loss. The latter occurs in long risers (tubing), even if the gas-rate at the bottom be kept constant. In order to analyze this type of instability, a simplified model of the phenomenon is required. The simplified model can be written using distributed delay models (as in the literature); also, it is possible to make a model using several artificial valves along the riser.

Tasks:

- a- Simulation of expansion driven instability in OLGA
  - b- Making simplified first principle or empirical model in Matlab
  - c- Comparing the results from OLGA and simple model
- \*There is a possibility to run experiments in multi-phase flow lab.

**Slug 2- Simplified first principle model for severe-slugging flow in S-shaped risers**

There has been a lot of research for modeling and control of L-shaped risers, and it has been assumed that behavior of S-shaped risers is not very different from the L-shaped ones. However, an S-riser has two bends and dynamics of the system are slightly different. We aim to investigate differences in behavior of two types of risers. We could use the model for L-shaped risers for S-shaped risers; otherwise we can extend the model for L-shaped risers by adding one more artificial valve for the second bend.

Tasks:

- a- Simulating S-riser in OLGA (one OLGA case for S-riser exists)
- b- Extending the simplified model for L-riser to S-riser
- c- Comparing the results from OLGA and simple model
- d- Comparing results from the S-shaped riser to results from L-shaped riser model
- e- Verifying the simplified model by experiments on the S-riser in multi-phase flow lab

**Slug 3- Configuration of two control valves for anti-slug control**

One topside choke valve has been used as the only manipulated variable for anti-slug control so far. But when we have two valves, an extra degree of freedom should make the control of the system easier in principle. We can investigate this by dynamic simulations and experiments.

We can use two control valves at the topside in series or parallel configurations; also, we can move one control valve to the riser base and compare its performance to that at the topside.

Tasks:

- a- Modifying the simplified model for adding the second valve at riser base or topside
- b- Controllability analysis based on the simplified model
- c- Dynamical simulations of control in Matlab and OLGA
- d- Running experiments on lab set-up at Chemical Engineering Department (K4, 3<sup>rd</sup> floor) laboratory.

#### **Slug 4- Modeling and simulation of severe-slugging flow using LedaFlow<sup>®</sup>**

OLGA has been our rigorous reference model for modeling of the severe-slug flow so far, and LedaFlow<sup>®</sup> is a newly developed competitor of OLGA. The behavior of LedaFlow software for severe-slug flow should be investigated; we are expecting the new tool will give more realistic results compared to OLGA.

**Supervisor: Professor Sigurd Skogestad, Co-supervisor: Esmaeil Jahanshahi (PhD student)**

#### **12: Optimization of processes using “self-optimizing” variables**

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

Steady-state simulation and optimization of LNG processes is difficult because of tight integration and small temperature differences between the streams. For example, the UniSim has large problems in converging when trying to optimize the operation of a given network. One possibility is to let Matlab do the optimization and UniSim the simulation. The focus in this project is on finding the best variables to specify in UniSim. Another approach is to use dynamic simulation for finding the steady-state solution. Also in this case the selection of good “self-optimizing” variables is critical.

**Co-supervisor: Vladimiros L. Minasidis (PhD student)**

#### **13: Dynamic back-off for control of active constraints**

To operate processes safely generally there are constraints which have to be observed. A typical examples for a safety constraint is the maximum allowable temperature in a reactor. Exceeding this constraint can lead to serious consequences, e.g. explosions.

At the same time, it often happens that the plant profit is maximised when a variable is at this constraint. Therefore it is desirable to operate the process as close to the constraint as possible. In practice, we will always have to back off a little bit from the constraint, because we want to make sure that we do not violate it, even if the the process conditions vary. At the same time, we want to minimize the back-off, because it causes economic loss.

The goal of this project is to study how the back-off can be adapted to dynamically changing operating conditions. The principal idea is to impose large back-off when the variable value changes fast, and little back-off when the variable changes slowly or not at all.

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

The tasks are

1. Literature review
2. Set up a small dynamic model
3. Find a law which dynamically adapts the back-off to the rate of change in the variable
4. Simulate a batch reaction process as a case study

**Co-supervisor: Jophannes Jäschke, postdoc**

#### **14: Flexible/optimal steady-state backoff for unconstrained variables to avoid infeasibility**

To operate processes safely generally there are constraints which have to be observed. A typical examples for a safety constraint is the maximum allowable temperature in a reactor. Exceeding this constraint can lead to serious consequences, e.g. explosions.

Variables which are unconstrained under a certain set of operating conditions may reach a constraint under other conditions. To remain truly optimal in both operating conditions, the control structure has to be changed.

In practice, however, one would like to keep the control structure simple and to use one control structure for all operating conditions.

This project involves investigating under what circumstances a control structure can be found, which may not be truly optimal, but which does not have to be adapted to changing constraints. We will consider the case of a linear plant and a quadratic objective function.

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

Tasks:

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

**Co-supervisor: Jophannes Jäschke, postdoc**

#### **15: Studies on modelling and control of distillation columns**

(in cooperation with Statoil/Gassco at Kårstø). Several projects possible. Need to be further discussed with Marius Govatsmark at Statoil Kårstø.

#### **16: Expected problems when pairing on negative RGA-elements**

The basis for this project is that it is not clear what happens if one pairs on a negative RGA. This will be a mix between simulation (in Simulink) and theory.

Background: Pairing on a negative steady-state RGA-element may give good decentralized control performance, but there are potential risks.

First, note that if one pairs on a negative RGA, then one cannot tune the controllers using independent designs (where each loop is tuned separately with the other loops in manual), because one would get instability when all loops are closed.

Second, consider sequential loop closing, which is probably more common practise. In this case, pairing on a negative RGA is claimed to result in instability, and the objective of this work is to study this in more detail.

**Project proposal: Professor Heinz Preisig: [heinz.preisig@chemeng.ntnu.no](mailto:heinz.preisig@chemeng.ntnu.no)**

#### **1: Temperature distribution in milli-reactor**

FluiTec is a small, hi-tech company located in Switzerland who is the innovator of a new reactor concept called ContiPlant. It is a Lego-like idea in which milli-reactors are the building blocks. These reactor types are currently tested by the large polymer industries to construct small-scale productions that can be placed into containers and thus are mobile. Production range is in the 10 k tons per year.

FluiTec is providing us with a reactor and together we build in a cutting edge temperature sensor which is based on an optical laser-inferential meter to measure temperatures along the axis of the reactor on at least 10 positions with only one fibre. The fibre is less than in the order of 0.2 mm and

the reactor inside approx 6 mm. So we are talking very highly sophisticated reactor equipment with highly sophisticated measurement equipment. We shall aim at constructing a dynamic residence-time distribution experiment for research and felles lab.

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

## **2: Residence-time distribution in various mixed systems**

As part of the renewal of the felles lab, I am extending the scope of reactor-engineering related projects. In particular the concept of residence-time distribution is being one of the targets. We are building a flexible bench-scale experiment, which demonstrates the hydraulic behaviour of various different physical systems. One of them is a hi-tech static mixer, but we shall extent also into sequences of tanks.

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

## **3: Continuous distillation**

We are nearly getting to finish the installation of a new distillation arrangement for the felles lab. New is essentially everything besides the centre column pieces: boiler, head, physical arrangement, a reflux pump, a flow measurement, control.

What we like to do is to refurbish two columns with additional pumps to enable them running in continuous mode. The pump arrangement is new as we built the pumps ourselves from commercially available components. There are new mechanical ideas we also discuss to replace the commercial pump head with a new advanced design.

Effort focus can vary from control, software to more engineering-type activities.

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

## **4: Colloid chemistry experiment**

I got a suggestion for a new experiment and would like to build it.

**Supervisor and daily contact: Collaboration with colloid group**

## **5: Chemical Engineering ontology for standard reactor types**

I am working on mapping chemical engineering into software which is using a framework called ontology. These beasts are the formal representation of concepts and rules underlying the models. So it is a type of concise representation of chemical engineering here limited to standard hydraulic reactor types. This may extend to work with TetraPak's engineering division that builds the world's biggest dairy manufacturing processes. The project aims at enhancing and partially substituting the current chemical engineering simulator software.

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

## **6: Computer-aided modelling**

We are building on a new tool expanding on three previous generations of modelling tools.

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

The project could be any combination of the following:

- use the existing theory definition tool to include the main balances (mass, energy, momentum)
- explore the possibilities of using the tool for distributed systems.
- implement thermo component
- expand to include entropy

Recent publication: <http://dx.doi.org/10.1016/j.compchemeng.2010.02.023>

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

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

### **7: Control and Felles lab rejuvenation**

The department received 2.5 million NOK for the development of the felles lab and the control lab. The control lab shall be updated and augmented with a couple of experiments. Initial plans have been developed. We invite to help thinking about possible, interesting processes and their realisation.

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

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

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

### **8: Automatic Safety and Hazard Analysis**

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

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

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

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

### **9: Simple Thermo Server**

The Process Systems Engineering group is heavily involved in process modelling particularly distillation. Distillation models and associated material models are used at a high frequency.

The project is aiming at implementing a server that provides:

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

The material model software is running and we are using it in a variety of ways. We thought it would be fun and very useful to build a little user interface that enables the interactive use of what the core can generate. This could then be put on-line in the form of a web page, for example. We have a rather generic distillation column model that is quite generally parameterised, which could be augmented with an appropriate interface to make it usable on the web.

Such a system has been realised for Yara. A prototype sever exists and is currently operable for ammonia, nitric acid and urea production. The Matlab interface is already working and we are working on an interface to other computer languages such as Python.

An interesting task would be to use an interface to gProms.

**Supervisors: Heinz A. Preisig, Tore Haug-Warberg**

### **10: On time scaling in chemical processes**

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

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

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

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

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

### **11: Frequency Analysis of Distillation**

Counter current processes show some very peculiar behaviours in the frequency domain. We have been analysing these behaviours in a couple of projects in the past: Ma, PhD on distributed models for tubular heat exchangers and the derivation of simple, but very accurate dynamic models. The findings have been verified in an experimental work done as a master thesis.

Recently we found a similar behaviour in distillation columns, which we would like to explore some more. Currently a project is ongoing looking into what looks like a simple linear counter current process, which has a structure similar to a distillation. This work should be continued towards a true distillation model. The work has potential to uncover a new methodology for identifying the internal dynamics in columns. It is thinkable that experimental work to that extent is added using the new-to-be-build columns in the felles lab.

Recent work: Puschke's diploma thesis available on request.

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

### **12: Process Identification using Wavelets**

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

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