CAPEC

PROCESS Industrial Consortium Research Report – 2014

Gani, Rafiqul; Woodley, John

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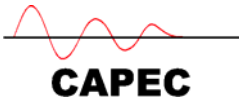
CAPEC-PROCESS Industrial Consortium
Research Report – 2014

Rafiqul Gani & John M. Woodley

June 2014



Department of Chemical & Biochemical Engineering
Technical University of Denmark
DK-2800 Lyngby, Denmark

http://www.capec.kt.dtu.dk
http://www.process.kt.dtu.dk

Preface

This report provides an overview of our research activities and achievements for the period June 2013 to June 2014. An overview of the active research projects is provided in terms of PhD-projects, post-doctoral and other research projects. A brief overview of the CAPEC-PROCESS software is also included in this report.

While CAPEC and PROCESS remain as independent centers, research results from both of the two centers are made available to the member companies of the consortium. In this way, the consortium members get access to a larger number of MSc- and PhD-projects as well as post-docs than before.

During the last 12-months, a number of PhD-projects have been successfully completed, while a number of new projects have been started. More specifically, the following PhD-students successfully defended their PhD-theses - within CAPEC: Alberto Quaglia (PEC13-41), Amol Shivajirao Hukkeriker (PEC13-42), Anne Katerine Vangsgaard (PEC13-50), Klaus Reinholdt Nyhuus Hansen (PEC14-10) and Nor Alafiza Yunus (PEC14-19); within PROCESS: Joana Lima Ramos and Aleksander Mitic; and, within PROCESS-CAPEC: Naweed Al-Haque (PEC13-35). By the end of 2014, Michele Mattei, Deenesh K Babi and Kresten T Meisner will be finishing their PhD-studies. At the same time, new PhD-students (Amata Anantpinijwatna, Rohana Abu, Marie Andersen, Ricardo Boiocchi, Maria Gundersen Deslauriers, Carina L Gargalo, Timo Hagemann, Seyed S Mansouri, Emmanuel Papadakis, Daniella Quintanilla, Caterina Seita, Anjan K Tula, and Andreas Åberg) have started their PhD-projects at CAPEC and PROCESS centers while 2 new post-doctoral projects were also started (Negar Sadegh and Nina M Andersen). Two visiting PhD-students, Pichayapan Kongpanna from Chulalongkorn University and Kosan Roh from KAIST came for extended stays of 12 and 6 months, respectively.

Collaborations with our member companies continue to help us to apply our research results to interesting industrial problems, to get valuable feedback on our methods & tools and to plan our future projects. Collaborations with our friends from academia help us to develop more comprehensive CAPE/PSE methodologies and techniques. We appreciate these collaborations and we thank our industrial and academic partners for their valuable contributions. During the last 12-months, we have finished a project with AstraZeneca and continued our collaboration with Alfa-Laval from our consortium members, and, Univ of Lorraine (France), KAIST (Korea), PROSPECT-UTM (Malaysia), UAM-C (Mexico), Chulalongkorn Univ-PPC (Thailand) and Univ of West Virginia (USA).

We would like to acknowledge the financial support in the form of membership fees from our member companies. No new company joined the consortium during the last 12 months but Conoco-Phillips left the consortium. For funding of PhD and post-doctoral research projects we would like to thank the Danish funding agencies FTP, EFP, DSF and ATV and the EC-research programs under FP7. Also, we would like to thank the governments of Malaysia, Brazil, Mexico, Korea and Thailand for sending students with PhD/MSc-scholarships.

Finally, we take this opportunity to thank all co-workers of CAPEC and PROCESS for their hard work and dedication. The research results highlighted in this report are their achievements. This is the 17th year since CAPEC and the industrial consortium were established.

For more information about the CAPEC-PROCESS consortium, please contact Mrs Eva Mikkelsen (eva@kt.dtu.dk), or Mrs. Gitte Nielsen (gnie@kt.dtu.dk).

Rafiqul Gani & John M. Woodley 1 June 2014

CONTENTS

1. Introduction

1.1 The CAPEC Center

Research at CAPEC is organized in terms of six research programs (see *Fig 1.1*). At the inner most level (research programs A, B), the topics are related to funda- mental research while at the outer most level (E), the topics are related to applied research. In the intermediate levels (C, D), systematic model-based algorithms, methods and tools are developed by em- ploying the results from the inner levels for use in applied research in the outer level. Since all research programs need numerical tools and databases, research program F supplies this need to all levels.

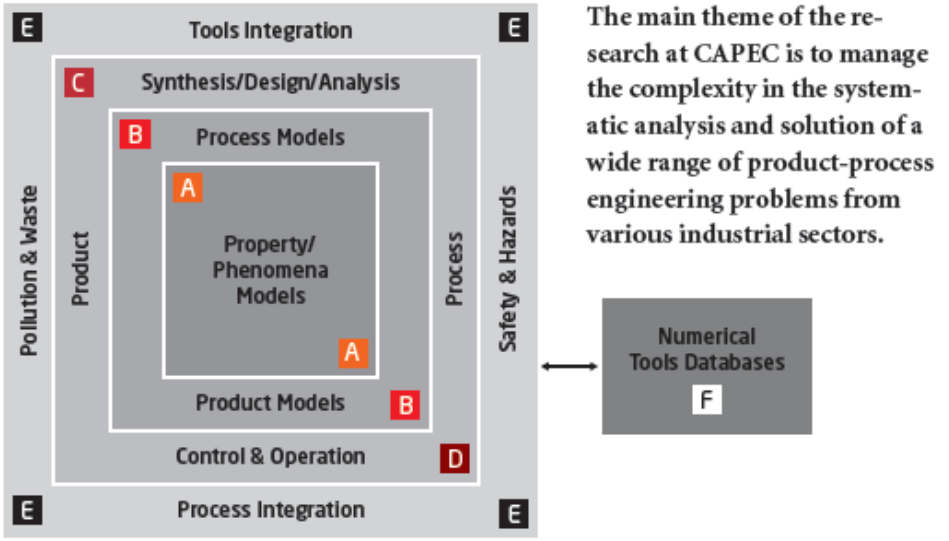


Figure 1.1: Organization of research in CAPEC in terms of research programs

Research

The six research programs are briefly described below:

- *Research Program A – Property and Phenomena Modelling*: deals with theoretical studies of properties (pure component and mixture) of chemical systems and phenomena such as permeability through membranes, reaction kinetics and mass transfer through diffusion. A library of group contribution based models for a wide range of properties of organic chemicals is one of the highlights of program A.
- *Research Program B – Process-Product Modelling and Simulation*: deals with the development of models and model-based simulation systems for prediction of the behaviour and performance of a wide range of chemical and biochemical processes (operating in batch, fed-batch and continuous modes) and a wide range of chemicals based products. A computer-aided modelling system for efficient model development and a collection of process-product models of various types, forms and scales are some of the highlights of program B.
- *Research Program C - Synthesis, Design & Analysis*: deals with the development and use of systematic algorithms, methods and tools for synthesis, design and analysis of chemical and biochemical processes and chemicals based products. Techniques such as computer aided molecular and/or mixture design (CAMD), and, process flowsheet design (CAFD) using the reverse approach are some of the highlights of program C.
- *Research Program D - Process Control, Operation & Monitoring*: deals with the development of use of systematic algorithms, methods and tools for process control, operation and monitoring, including process analytical technologies. Techniques for tuning of controller parameters in model predictive control and methods for design of PAT systems are some of the highlights of program D.

- *Research Program E - Process and Tools Integration*: deals with on-line (process) and off-line (tools) integration as well as safety & hazards, sustainability analysis, and integration of process design-control, process-product design and process-process. Integrated software such as ICAS, virtual process-product design lab, SustainPro and their associated methodologies are some of the highlights of program E.
- *Research Program F - Database and Numerical methods*: since the CAPEC-PROCESS software needs to be self-sufficient in all respects for use by the industrial consortium companies, CAPEC also maintains a library of numerical methods and databases (properties of chemicals and solvents, reaction synthesis, membranes, and analysis equipments). The other research programs benefit from this in terms of data for modelling and improved simulation strategies.

Based on the above, the research objectives of CAPEC are summarized as:

> *Develop computer-aided systems for efficient and reliable process simulation; for systematic synthesis, design and analysis of sustainable chemical products and their manufacturing processes; for robust control, operation and monitoring of processes from principally chemical, petrochemical, pharmaceutical and biochemical industries. The computer-aided systems are to be developed based on fundamental and/or data-based modelling studies that incorporate correlation and estimation of thermo-physical and phase equilibrium properties as well as modelling the underlying principles / behaviour of the process-product. That is, by managing the complexity in a systematic and efficient manner.*

CAPEC's research is focused - while the application horizon is wide (oil and gas, petrochemical, chemical and specialty chemical, pharmaceutical, food and bio industrial sectors) the focus is on the use of a systems approach. CAPEC's strengths in terms of its research focus - pioneering work in certain research areas (such as modelling; methods for synthesis, design and analysis of process as well as products; process and tools integration), industrial collaboration (dissemination of research results through the industrial consortium as well as collaboration with academia), and contacts (ability to influence developments within chemical engineering and CAPE/PSE). More specifically, CAPEC's contribution in the areas of thermodynamic property modelling for process-product design; computer-aided molecular-mixture design for consumer product development; targeted reverse approach for process intensification and integration; systematic computer-aided methods and tools for modelling, design, analysis and control are well known within the CAPE/PSE community.

Personnel

CAPEC's permanent staff comprises Head of Center Professor Rafiqul Gani, Associate Professors Gürkan Sin and Jens Abildskov, Professor (Docent), Karsten Clement, Assistant Professor Jakob Kjøbsted Huusom and Secretary Eva Mikkelsen.

Industrial Consortium

CAPEC has established an industrial consortium, where the PROCESS group is also involved. Through the industrial consortium, CAPEC-PROCESS coworkers have the unique opportunity to get quick and useful feedback on their developed models, methods and tools as well as insights to the current and future needs of the various industrial sectors represented by the consortium members (see 7.4 for a complete list of the CAPEC-PROCESS member companies).

Dissemination

The dissemination of the research results of CAPEC is carried out in terms of:

- *Computational Tools*. Predictive models for reliable property estimation for a wide range of chemicals; generic mathematical models for process operation, product performance;

computer-aided tools for product-process synthesis & design, etc., are used by leading industries and close to 75 universities from all over the world.

- *Technology*: Developed systematic methodologies for process-product synthesis, design, analysis and control (& operation), simulation strategies, solvent selection (& design), pollution prevention, sustainable process-product alternatives, etc., are routinely used to solve industrial problems and in education.
- *Application*: Industrial case studies, tutorial case studies, technology transfer studies and consulting.

Activities

The activities shown in *Table 1.1* highlight the scope and significance of the research results available to the CAPEC-PROCESS industrial consortium members in terms of the industries where the developed methods and tools are applicable.

Table 1.1: Scope and significance of CAPEC research results shown in terms of industries where they can be applied.

CAPEC Research Programs	Application of Research Results in terms of Industry					
	Petrochemical[1]	Chemical[2]	Pharmaceutical	Agrochemical	Bio & Food	Aroma
Models & modelling tools						
Synthesis, design analysis & evaluation						
Control, operation & monitoring						
Process & tools Integration						
Databases & Numerical Methods						

[1]: Includes also oil & gas industries; [2]: includes also specialty chemicals

Work done during 2011-2012

More focus given in these areas

Well-developed methods & tools available*

Available methods & tools can easily be adapted if not directly applicable*

Available methods & tools applicable to only a small number of problems*

Needs development

*Solving problems in process modelling, simulation, design, analysis and control

Some of the challenges for the future are to use our methods and tools to find more sustainable alternative routes for the production of important chemical products in the petrochemical and chemical sectors using renewable and/or newly established resources; to help in the sustainable design/development of new and improved chemicals based products and the processes that manufacture them for the pharma, bio-food, agro and aroma industrial sectors; and, to incorporate in all problem solutions the issues related to energy, water, environment and green chemistry.

CAPEC is currently involved in the following large collaborative projects in Denmark and also outside Denmark.

- OPTICO project: This is a EC-funded research project in the area of modelling and process intensification. CAPEC has received funding equivalent to 48 man-months of funding for researchers. The project started in January 2012 and ends in January 2015. The objective of the project is to develop model based methods and tools in the area of process intensification.
- QNRF: This is a project funded by the Qatar National Priority Research Program. The objective is the design of synthetic fuels and value added chemicals derived from natural gas via

combined experimental and process integration methodology. The project started in December 2012 and will end in 2015 with the Texas A&M University at Qatar, the Texas A&M University at College Station (Texas) and CAPEC as partners.

- EcoDesign MBR: The Danish Council for Strategic Research has founded the EcoDesign MBR Centre in the period from 2010-2016 together with companies and universities. As project partner, CAPEC received funding for 1 PhD and 1 postdoctoral researcher in the area of developing membrane bioreactor (MBR) based technology for wastewater treatment. CAPEC will be developing process modeling to support technology development including design, optimization, operation and control as well as model-based tool for bioprocess scale-up to full-scale applications.
- SWI: Storm- and Wastewater Informatics "SWI" is a strategic Danish Research Project funded for the period of 2008-2012 with an overall aim to close the knowledge gaps within prediction and control of current and future conditions in integrated urban wastewater systems. CAPEC received funding for 1 postdoc. As part of this project, CAPEC also received an industrial PhD funding from FTP the period 2011 – 2014. The project will develop optimizing control for integrated sewer and wastewater treatment plant systems.
- RENESENG – Renewable Systems Engineering: This new Marie Curie ITN project was recently awarded to a consortium including CAPEC. RENESENG aims to prepare a new generation of highly qualified researchers in biorefinery and biobased chemicals. CAPEC will train two early stage researchers in the area of sustainable process design and development of computer aided process synthesis methods and tools.
- THERMCYC – This project is funded by the Danish Strategic Fund (DSF) and deals with selection, design and analysis of heat-pump systems. CAPEC's contribution is two PhD projects and 30 man-months of post-doc. The project started from1 January 2014 and its duration is 5 years.

1.2 The PROCESS Center

The Center for Process Engineering and Technology is focused on the development of new and innovative production processes for industry. PROCESS works at the interface of a number of disciplines, including chemical engineering, biotechnology, process engineering and chemistry. The objective is to provide the necessary infrastructure and support to evaluate and implement the next generation of processes in the chemical, bio-based and pharmaceutical sectors in particular. All research is carried out in close collaboration with industry and work is carried out at three levels, namely: laboratory scale experimental process evaluation; model based evaluation of process technology and pilot-scale and full-scale process validation. Two demonstration units operate in the pilot facilities (both for immobilized and soluble enzyme reactions at 10-20L scale), and specifically for fermentation experimental work at large scale is performed in close collaboration with industrial partners. Using the results from work at the three levels enables new technology and processes to be evaluated both experimentally and also from the perspective of implementation, including economic and environmental evaluation. The research is divided into 3 research areas:

Main research areas:

1. Experimental-based product-process synthesis, design & analysis. With focus on micro-scale devices and processes – the development of miniaturised unit operations and processes, both to collect data rapidly and in parallel of use for modelling, and also to develop modular process screening tools.
2. Biocatalytic processes – the development of enzymes (and whole-cell) based processes where high selectivity and mild conditiopns are required. The focus is especially on multi-enzymatic and chemo-enzymatic processes. Downstream processing and product recovery are integrated in all processes.

3. Fermentation technology – the development of improved understanding of fermentation processes operated at large-scale, using tools such as computational fluid dynamics (CFD) combined with experiments. Development of improved monitoring and control strategies for fermentation processes.

The PROCESS Center is involved in a number of collaborative projects, both in Denmark and in Europe. Examples of large collaborative projects with participation of PROCESS are:

- PROCESS is one of the partners in P4FIFTY, an FP7 funded European Marie Curie Training network (ITN) of academic and industrial researchers looking to develop enzymatic methods for green oxidation chemistry through the isolation, redesign and application of cytochrome P450 enzymes.
- A new FP7 project (BIOINTENSE) has started in 2012. It is focused on a micro-scale approach for the rapid development of biocatalytic processes. PROCESS is the project coordinator.
- PROCESS has joined the SANITAS project, an EC-funded project (ITN) with focus on the development of the next generation of modelling and simulation tools for performance evaluation of wastewater treatment plants.
- PROCESS has started the EUROMBR project, a Marie Curie FP7 ITN with focus on the development of miniaturized experimental tools for studying biocatalysis and fermentation processes. PROCESS is the project coordinator.

The vision of the Center for Process Engineering and Technology is to provide the necessary support to enable the next-generation of processes to be implemented in industry. In this way the new developments in biotechnology, catalysis and separation science alongside process engineering can be translated into industrial practice. New processes with reduced waste, high efficiency and based on all the principles of sustainability can be developed which will help develop the European industrial sector in the production of chemicals, bio-based materials and chemicals, as well as pharmaceuticals.

1.3 CAPEC-PROCESS Activities

While maintaining their unique center activities, it has been decided to join forces on a set of research topics of mutual interest within the pharmaceutical, agrochemical and bio & food industrial sectors. The interaction between the CAPEC and PROCESS centers at the level of the industrial consortium is illustrated through *Fig 1.2*. For the industrial consortium, the CAPEC-PROCESS collaboration should result in increased data-knowledge on chemicals based products and their processes, design of the product-process, control-monitoring of the product-process, and, development of more sustainable and "greener" products-processes. The two centers tackle these problems from two different approaches: CAPEC employs a model-based systems approach that also leads to computer-aided tools, while, PROCESS employs a systematic experiment/data based process understanding to perform the necessary process analysis and evaluation. The CAPEC-PROCESS collaboration therefore is able to generate methods and tools that are not only able to provide new innovative product-process designs but can also provide fundamental understanding, analysis and evaluation of the design problem. This is essential for future implementation of these processes in industry.

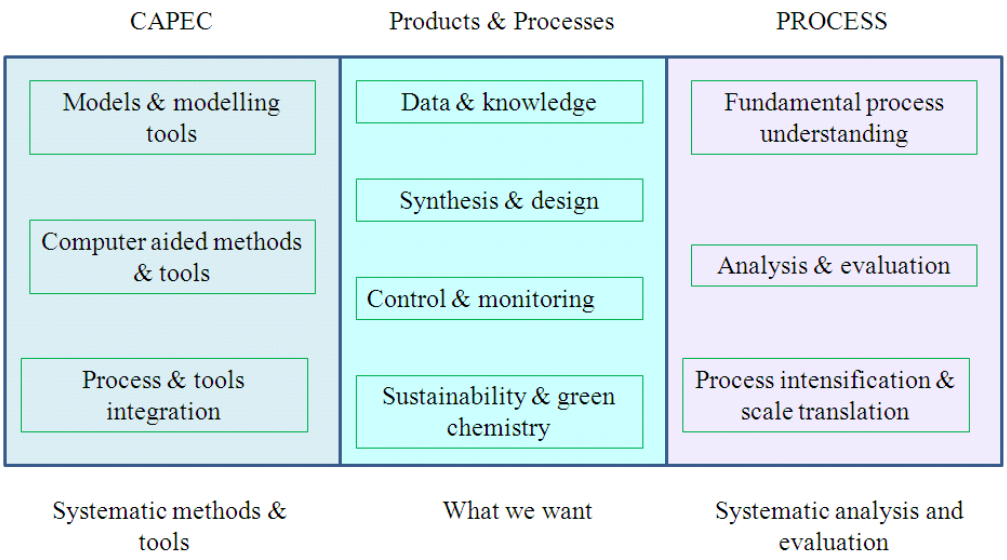


Figure 1.2: Collaboration between CAPEC and PROCESS centers

1.4 Research Highlights

One research project from each center is highlighted below. From CAPEC, its project on computer aided modelling is highlighted. From PROCESS its project on fermentation technology is highlighted. Also, the process intensification research area is highlighted where PROCES and CAPEC have collaboration.

1.4.1 CAPEC: Computer Aided Modelling

Models play important roles in design, operation and analysis of chemicals based products and the processes that manufacture them. In the area of product-process design, the problems differ in terms of the type of chemical(s) being produced. The products and the processes that make them, from petrochemical and chemical industries are usually commodity chemicals produced in large amounts. In this case, process optimization in terms of operational efficiency and cost is usually a defining factor for a candidate product-process. The products from life sciences, pharmaceutical related industries, on the other hand, are usually large and/or complex molecules, produced in small amounts. Here, process optimization in terms of operational reliability and time of operation is usually a defining factor. This means that although the steps in the systematic solution of different types of problems could be the same, the models and data, and the methods and tools that employ them in the various solution steps may be very different.

The need for systematic model development tools in terms of model definition, model evaluation, model analysis, model verification and model validation is gaining more attention with increasing demand for model-based methods and tools. However, when the required models may be complex, and require as well, multiple time and/or length scales, their development and application in various types of problems is not trivial. Therefore, a modeling framework with the associated tools can contribute by reducing the time and resources needed for model development and application, thereby reducing the overall time and cost for product-process development.

The development of methods and tools that will allow systematic generation, analysis and solution of models for various objectives is the goal of this project. The first version of a computer-aided modeling framework integrated with systematic model derivation and associated modelling tools have been developed (see *Fig 1.3*). The framework includes features for model development, model identification and solution, and, a library of model templates. Current and future work is looking at

increasing the number of problem-specific models that can be developed from model templates available in libraries. Also, further development of computer-aided tools for implementation of two-ways connections between available tools in the framework and export of models to external software, including transfer of models in formats such as xml, Matlab (m-file) and CAPEOpen are being investigated.

The modeling framework also contributes to other projects in CAPEC and PROCESS that require the development and use of models.

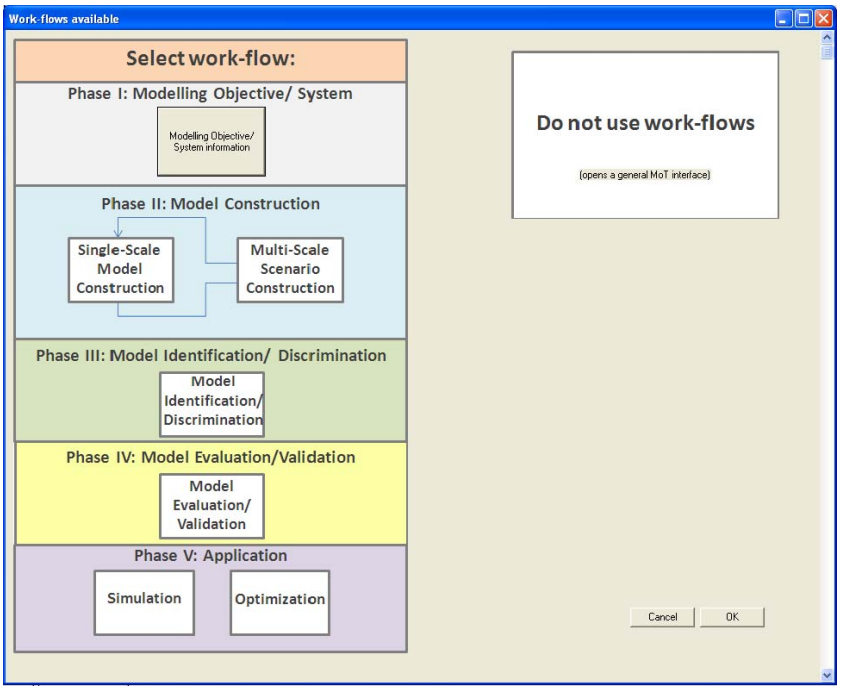


Figure 1.3: Representation of the computer aided modeling framework

1.4.2 PROCESS: Industrial Fermentation Technology

A professor position to promote and further develop Industrial Fermentation Technology as a research area has been established with support from Novozymes A/S (Denmark). Krist V. Gernaey has been appointed professor at DTU Chemical Engineering from 1 January 2013 onwards. Krist received a MSc degree from Ghent University, Belgium in 1993 and a PhD degree in Applied Biological Sciences from Ghent University as well in 1997. He has been employed as Associate Professor at DTU Chemical Engineering from August 2005 onwards. Krist has been active within the Center for Process Engineering and Technology (PROCESS) from January 2010 onwards, as co-founder of the center, and in close collaboration with Prof. John M. Woodley.

A strong development in the field of industrial fermentation technology in the coming years can now be expected, and that these activities will be advantageous for the consortium. In 2013, four PhD projects have been started related to industrial fermentation technology. New research activities, in close collaboration with industry, will combine experimental fermentation work at different scales with mathematical models and a detailed physiological understanding of the microorganisms. Due to the close collaboration with Novozymes A/S, DTU Chemical Engineering will have access to industrial scale reactors, both with respect to performing experimental work and process characterization on the one hand, but also with respect to the practical testing of new ideas that might result from the research work at DTU on the other hand. This is a rather unique situation, and will be a major advantage for the development of the field at DTU Chemical Engineering.

More specifically, the aim is to work with research on:

- Mass transfer in large tanks / characterization of spatial heterogeneity in large tanks
- Microbial physiology
- Scaling up/down, supported by Computational Fluid Dynamics (CFD)
- Modelling / monitoring of fermentation processes
- Scaling down: further development of parallel ml-scale reactor platform
- Novel sensors and control, e.g. Raman spectroscopy applied to fermentation, use of soft sensors for prediction of variables of interest
- Rheology of biomass suspensions, e.g. to link the morphology and structure of microbial aggregates with the viscosity of the fluid/fermentation broth
- Heterogeneity: development of a better understanding of the heterogeneity in a population of cells, and how interactions with spatial heterogeneity influence this population heterogeneity

The first PhD project in the area has been started already in January 2013, under the umbrella of the BIOPRO project and in close collaboration with the companies Novozymes A/S and Novo Nordisk A/S. Anders Nørregaard has been hired as the PhD-student and the project will focus on improving our understanding of mass transfer in large scale aerobic fermentations, combined with investigating different ways of operating such fermentations in a more efficient way. Also in 2013, a new PROCESS lab has been established that will allow us to perform lab-scale fermentations.

1.4.3 CAPEC-PROCESS joint project in Process Intensification

The objective of process synthesis is to find the best flowsheet, among numerous alternatives for converting specific raw materials to specific desired products subject to predefined performance criteria. The unit operations concept is the one most used for process synthesis because it allows one to associate the operational tasks with the the necessary processing route. This concept has been successfully applied for decades and continues to be applied in the various industrial sectors. However, due to increasing demands on the chemical industry to reduce waste, to reduce environmental impact, to increase use of renewable resources, etc., one has to question if new and innovative solutions that can make a difference are being obtained? The problem here is that when applying the unit operations concept one automatically connects the unit operations with their function and therefore this mode of thinking restricts the solution space to only a limited number of 'well defined' unit operations. Through process intensification, it is possible, in principle, to create new unit operations if the operational tasks are analyzed at the phenomena level rather then the usual unit operation level. Incorporating as well, a sustainability analysis within the process synthesis framework helps to identify process-operational bottlenecks that can be addressed through intensified operations.

Within this project a computer-aided framework for process synthesis has been developed that helps to develop a sustainable (and intensified) design of a chemical process. New chemical and/or biochemical processes can be synthesized and intensified as well as existing ones. The method is generic in terms of the solution steps and tools used but system specific in terms of models used to represent them.

Two PhD-projects and several MSc-level projects have been started within this research area. Biochemical processes (such as sustainable production routes for biodiesel) as well as chemical processes are being analyzed and improved in terms of sustainability through intensified process alternatives. A number of computer aided tools (SustainPro, ECON, LCSoft, etc.) have also been developed for use through the framework.

The Department of Chemical & Biochemical Engineering at the Technical University of Dortmund and the Department of Chemical Engineering at Auburn University are international collaboration partners in this project.

2. Organization of Activities

The organization of educational and research activities within CAPEC and PROCESS are conducted by the faculty members of the two centers together with the researchers and students associated with them. *Fig 2.1* highlights these activities, where it can be noted that the research results coming out of the six research programs of CAPEC-PROCESS are disseminated in education and industry.

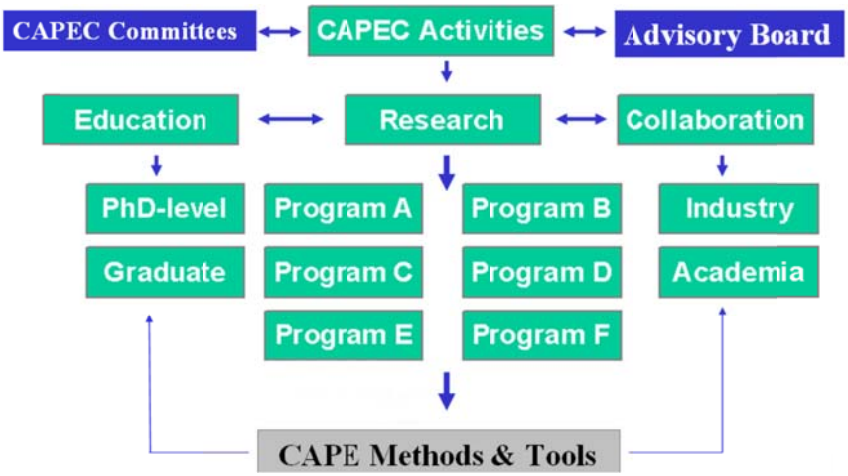


Figure 2.1: Organization of educational and research activities within CAPEC.

2.1 Permanent Members

CAPEC	
 **Assistant Professor Jakob K Huusom (JKH)**	The primary research area is process operation and control. Specific activities are related to: • First principle modelling and simulation of dynamical systems related to the chemical and biochemical industry. • Parameter estimation in dynamical systems. • Chemical and biochemical plant monitoring and operation. • Plant wide control. • Optimal control and state estimation. • Modelling and estimation for process control. • Tuning and maintenance of control implementations. Current projects are related to applications within: Diabatic distillation; automotive flue gas cleaning; and enzymatic production of biodiesel. ***Research Areas (CAPEC):*** *B, D, E*

Associate Professor Jens Abildskov (JA)

Research focuses on development and analysis of correlations and predictive models for thermodynamic properties of fluids for chemical process design. Relationships are sought between molecular structure and thermodynamic properties for simple descriptions of thermodynamic properties. For densities and activities of strongly non-ideal fluids this is offered by statistical mechanical methods based on molecular correlation functions and their connections to fluctuation properties. Examples of applications are

- thermodynamic modeling and microscale simulation for properties relevant to biocatalysis
- mixed solvents (liquids and ionic liquids) with dissolved gases, enzymes and pharmaceuticals

Applications in process energy requirements to determine the efficiencies of diabatic distillation processes & reverse engineering.

Research Areas (CAPEC): *A, B, F*

Associate Professor Gürkan Sin (GSI)

The research, in general, focus on development of systematic methods and tools for understanding, design, operation and control (bio)chemical processes and aims at providing rationale basis for better informed decision-making in engineering applications to achieve energy efficient and sustainable chemical & biochemical industry. Current research aims at moving the current design paradigm to predictive and probabilistic-based approaches and includes:

- Model-based product-process design; technology evaluation, process synthesis & process retrofitting; effect of uncertainties
- Dynamics & process control; Integrated process design and control; plantwide control; model-based control and operability analysis; fuzzy-logic diagnosis and control;
- Process modelling; model identification; model analysis; numerical methods; systems approach
- Uncertainty analysis; Sensitivity analysis; Monte-Carlo simulations; Bayesian Inference; Variance decomposition;
- Process monitoring, safety and risk assessment

Applications in chemical, biochemical (biotechnology, fermentation technology, etc), pharmaceutical, food and water industries.

Research areas (CAPEC): *B, C, D, E*

Reader Karsten Clement (KHC)

KHC is the Director of BSc Study Program (Chemistry & Chemical Engineering). His research interests lie in process modelling and process control and operation.

Research areas: *B, D*

Professor Rafiqul Gani (RaG)

RaG is Director and Co-founder of CAPEC. His research areas of interest covers modelling (properties, process & product); product (molecular-mixture) design; process synthesis, sustainable design & analysis; process-tools integration; and, development of computer-aided systems. Some of the currently active research topics are listed below:

- Modelling (chemical products, processes and their operations; performance of products; properties of chemical systems)
- Synthesis, design and analysis of chemical products and their sustainable processes (CAMD and CAFD)
- Development of methods for sustainable process design; for process intensification; for integration of design-control; for model-based product quality control
- Development of integrated computer-aided systems (ICAS, PAT, SustainPro, Databases)

Applications in petrochemical, chemical, specialty chemical, agrochemical, food and pharmaceutical industries

Research Areas (CAPEC): *A, B, C, D, E, F*

PROCESS

Professor Krist V Gernaey (KVG)

KVG's main research topic is industrial fermentation technology. His main research activities at this moment are:

- Process scale-up and scale-down applied to fermentation processes, including use of Computational Fluid Dynamics (CFD) and population balance models (PBM) to study heterogeneity in fermentation processes
- Process modelling, applied to fermentation, biocatalysis, biological wastewater treatment, food production, pharmaceutical production, and biofuel / biorefinery processes.
- Design of new reactor systems, including microbioreactors for enzymatic reactions and fermentation + systems for continuous production of pharmaceuticals
- Process Analytical Technology (PAT) and Quality by Design (QbD). Including for example on-line monitoring of fermentation processes + continuous organic synthesis
- Benchmarking of control strategies for wastewater treatment plants

Research Areas (PROCESS): *1-3*

Professor John Woodley (JW)

JW coordinates research on biocatalysis and related process technology. His main research interests lie in the following topics:

- Technologies for the implementation of new biocatalytic processes, including *in-situ* product removal, novel reactors, biocatalyst recycle and integration with operating and control strategies
- Multi-step biocatalysis, including chemo-enzymatic conversions and multi-enzymatic conversion in cascades.
- Tools and methodlogies for the implementation of new biocatalytic processes, including strategies to achieve commercial targets and scale-up.

Applications in chemical, biochemical (e.g. biotechnology, fermentation technology, biofuel) and pharmaceutical industries.

Research areas (PROCESS): *1-3*

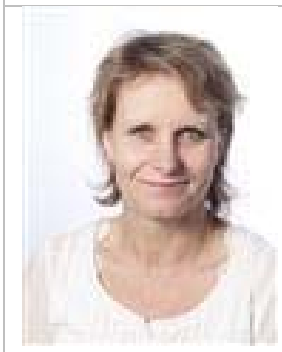
Associate Professor Ulrich Krühne (ULKR)

ULKR is coordinating the microfluidic research-development, which has gained significant importance in chemical engineering. Topics of research interest:

- Micro scaled fluid dynamic properties and their influence on chemical, biochemical and physical interactions
- Integration of different unit operations into a single step process
- Computational fluid dynamic methods

The research combines PSE activities with experimental investigations. A target area is the intensification of processes or reactor technology. This can be seen in the active interaction in European projects as well as within national research projects.

Research areas (PROCESS): *1-3*

CAPEC-PROCESS Secretaries	
 **Eva Mikkelsen (EVA)**	Eva is the administrative secretary for the CAPEC center and the CAPEC-PROCESS consortium. Eva also serves as the secretary for the editorial office of the Computers and Chemical Engineering journal office.
 **Gitte Nielsen (GNIE)**	Gitte is the administrative secretary for the PROCESS centers and the CAPEC-PROCESS consortium.

3. Research Projects

3.1 List of current research projects

Research at CAPEC & PROCESS is conducted through research projects at various levels: post-doctoral, PhD, MSc, BSc and visitor-collaboration projects. Table 3.1 provides a list of the currently active projects.

Table 3.1: Currently active research projects at all levels

CAPEC Post-Doc	Project Title	Supervisors	Start	End	Funding
Alberto Quaglia	Model-based upscaling of bioprocesses	GSI/RaG	9-2013	2-2014	EcoDesign

PROCESS Post-Doc	Project Title	Supervisors	Start	End	Funding
Miguel Mauricio Ingleisas	Advanced tools for easy(ier) control	KVG	02-2013	07-2014	BioPro
Xavier Flores-Alsina	New process models to simulate, benchmark and control urban wastewater treatment Systems	KVG	05-2013	04-2015	BioPro
Negar Sadegh	Modeling heat and mass transfer in industrial ovens used for baking	KVG			
Nina Marianne Andersen	Modeling and optimisation of an industrial filtration process	KVG			

CAPEC PhD Student	Project Title	Supervisors	Start	End	Funding
Michele Mattei	Systematic methodology for design of emulsion based chemical products	RaG/GK	8-2011	7-2014	DTU, CAPEC, CERE
Ane H. Mollerup	Optimizing control of the integrated urban wastewater system	GSI	8-2011	7-2014	Københavns Energi, FTP Industrial PhD
Larissa Peixoto Cunico	Modelling of phase equilibria and related properties of mixtures involving lipids	RaG/Sarup/ Cerriani	2-2012	1-2015	DTU, Alfa Laval
Marina Fedorova	Systematic Methods and Tools for Computer Aided Modeling	RaG/GSI	4-2012	3-2015	EU FP7 OPTICO project
Thomas Bisgaard	Operation and Design of Diabatic Distillation Processes	JA/JKH/ NVS/KP	9-2012	2-2016	DTU

Zainatul Bahiyah Binti Handai	Synthesis and Design of Water/Wastewater networks	RaG/GSI	6-2013	5-2016	Government of Malaysia
Sawitree Kalakul	Property Modelling and Process Design involving complex chemical systems	RaG/Sarup/ GK	6-2013	5-2016	DTU; Alfa Laval; Qatar Fund
Andreas Åberg	Modeling and Operation of Diesel Engine Exhaust Gas Cleaning Systems	JA/JKH	8-2013	7-2016	HTF/KT
Amata Anantpinijwatna	Generic model-based tailor-made design and analysis of biphasic reacting systems	RaG/GSI	8-2013	7-2016	Government of Thailand
Carina Loureiro da Costa Lira Gargalo	Sustainable design of biorefinery systems for biorenewables	GSI/RaG	11-2013	11-2016	FP7 RENESENG
Anjan Kumar Tula	Improved LCA methodology and software tool for biorenewable products and processes	RaG/GSI	12-2013	12-2016	FP7 RENESENG
Jérôme Frutiger	Computer-aided molecular design of novel working fluids to optimize heat transfer processes	GSI	6-2014	5-2017	THERMCYC

CAPEC-PROCESS PhD Student	**Project Title**	**Supervisors**	**Start**	**End**	**Funding**
Kresten Troelstrup Meisler	Multi-dimensional population balance models of crystallization processes	RaG/KVG/ NVS	3-2011	2-2014	DTU
Deenesh Babi	Phenomena based process intensification	RaG/JW	8-2011	7-2014	DTU, CAPEC, PROCESS
Jason Price	Operation and Control of enzymatic biodiesel production	JW/JKH	9-2011	8-2013	DTU
Hande Bozkurt	Computer aided framework for synthesis, design and retrofit of water networks in processing industries	GSI/KVG	12-2011	12-2014	DTU
Peam Cheali	Integrated framework for synthesis and design of multi-product biorefinery networks	GSI/RaG/KVG	5-2012	4-2015	EU FP7 OPTICO project
Seyed Soheil Mansour	Design, control and analysis of intensified biochemical processes	RaG/JKH/ JW	9-2013	8-2016	DTU/CAPEC/ PROCESS
Riccardo Boiocchi	Plantwide modelling and control for N2O from WWTP	GSI/KVG	10-2013	9-2016	DSF / LaGas
Emmanouil Papadakis	Modeling and Synthesis of pharmaceutical	RaG/GSI/	10-2013	9-2016	DTU

	processes: moving from batch to continuous manufacturing	KVG			

PROCESS PhD Student	Project Title	Supervisor	Start	End	Funding
Aleksandar Mitic	Operational aspects of continuous pharmaceutical production	KVG/KDJ	11-2010	11-2013	DTU/Lundbeck/MP2T
Laura Snip	Extending the BSM platform with occurrence, transport, and fate of micropollutants using the ASM-X framework	KvG/ULKR/ XAL	05-2012	04-2015	SANITAS
Marie T Andersson	Bioprocess engineering for the application of P450s	JW			
Søren Heintz	Mastering Process Intensification across Scales for ω-Transaminase Processes	KVG/JW/ULKR	09-2012	08-2015	BIOINTENSE/DTU
Rolf Hoffmeyer Ringborg	μ-Tools for Development of ω-Transaminase Processes	JW/KVG/ULKR	10-2012	09-2015	BIOINTENSE/DTU
Ines Periera Rosinha	Topology optimization in biocatalytic reactions using miniaturized	ULKR/JW/KVG	11-2012	10-2015	BioIntense/DTU
Hilde Larsson	Modeling and topology optimization of fermentation processes in microbioreactors	ULKR/KVG/ A. Ladegaard	12-2012	11-2015	Novo Nordisk Foundation
Anders Nørregaard	Mixing and oxygen transfer processes in bioreactors	KVG/JW/ULKR	01-2013	12-2016	BIOPRO/DTU
Rohana Abu	Design and Evaluation for Multi-enzyme Processes	JW			
Catarina Seita	Bioprocess Evaluation Tools	JW			
Maria Gundersen Deslauriers	Evaluation of thermodynamics for biocatalytic reactions for biocatalytic reactions	JW			
Daniella Quintanilla	Linking Strain Morphology to Rheology and Mass Transfer as a Means to Improve Fermentation Processes	KVG			

External PhD-Students	Project Title	Supervisor	Start	End	Funding
Pichayapan Kongpanna	Technological Evaluation of CO_2 utilization: Dimethyl Carbonate Synthesis	RaG	7-2013	6-2014	PPC Chulalongkorn, Thailand
Kosan Roh	Superstructure-based techno-economic feasibility study of CO2 conversion technologies for the methanol production	RaG	5-2014	11-2014	KAIST, South Korea

MSc-project Students	Project Title	Supervisor	Start	End	Funding
Yohann le Guennec	Study of liquid-liquid phase splits in complex mixtures of gasoil, ethanol and FAEE (fatty acid ethyl esters)	RaG	1-2014	6-2014	ensic.inpl-nancy
Rebecca Frauzem	Techno-economic evaluation of a CO2-conversion process	RaG	2-2014	8-2014	DTU
Stefano Cignitti	Computer-Aided Reaction Path Synthesis	RaG	2-2014	6-2014	DTU
Maria-Ona Bertran	Chemical processing routes based on reaction pathways	RaG	2-2014	7-2014	DTU
Caroline Gundorph Møller	Sustainable Alternatives for the Production of Methylene Diphenyl Diisocyanate	RaG	2-2014	8-2014	DTU

3.2 CAPEC-PROCESS research programs versus co-workers

An overview of the research programs and the CAPEC personnel involved with them is given in Table 3.2a and an overview of the research programs and the PROCESS personnel involved with them is given in Table 3.2b.

Table 3.2a: Overview of CAPEC personnel and their research topics

Research Programs	**CAPEC coworkers & research activities**				
	Faculty[1]	**Post-Docs**[2]	**PhD-students**[2]	**MSc-students**[3]	**Others**[4]
A: Property & Phenomena Modelling	**JA**; RaG	(*NAS)*	(*AZM*); (*NOY*); (*AMH*); LACU; MICU; *Sawit*	(*S Kalakul*)	Y LeGuennec
B: Product & Process Modelling	**RaG**; GSI; JA; JKH		(*NOY*); (*AQ*); (*AKV);* KreTM;JAPR; HBoz; MFad; PChe; Thbis;Molle; Zbha; *Amatana; Empap; Ricco; Calour; Seso; Antu*	M Bertram; S Cignetti; R Frauzem	K Roh
C: Synthesis, Design & Analysis	**GSI**; RaG		(*AZM*); (*NOY*); (*AQ*); KreTM; MICU; DKBabi; HBoz; PChe; Thbis; Zbha; *Ricco; Amatana*, *Sawit; Empap; Antu; JF, Calour*	(*C H Hansen*); C G Møller; M Bertram; S Cignetti; Thai-1	P Kongpanna
D: Control, Operation & Monitoring	**JKH**; GSI; RaG; (KHC)		(*NAS*); KreTM; JAPR; Molle; *Seso; Empap*		
E: Process & Tools Integration	**GSI**; RaG; JKH	*(AQ)*	(*AMH*); (*AQ*); (*AKV*); (*KRNH*); KreTM; DKBabi; HBoz; MFad; PChe; Zbha; *Sawit; Antu; Calour; Ricco; Seso*	(*S Kalakul*); R Frauzem; A Ruben; Thai-2	M Rizwan; P Kongpanna; K Roh
F: Databases & Numerical Methods	**JA**; RaG		(*AMH*); MICU; LACU; Thbis; *Sawit*	(*S Kalakul*)	
Currently active	**4**	**(*2*)**	**20**	**8**	**3**

1: Research area coordinators are indicated in bold; 6: New PhD-students who have started are indicated in italic; post-docs who have finshed are marked in italic-parenthesis 3: MSc-students who have finished are indicated by italic-parenthesis; 4: Here, visiting students (PhD, MSc, BSc) are listed, PhD-students are listed in italics. All other names indicate current coworkers at CAPEC-PROCESS.

Table 3.2b: Overview of PROCESS personnel and their research topics

Research Programs	**PROCESS coworkers & research activities**				
	Faculty[1]	**Post-Docs**[2]	**PhD-students**[2]	**MSc-students**[3]	**Others**[4]
1: **Experimental-based product-process synthesis, design & analysis.**	ULKR; JW; KVG	MMI; NES; ASMI; NMAN	VKB; HEMRA; MANDE; SHEIN; ROLRI; INROS; *CASSE; ROHA*; *ASTP*		
2: Biocatalytic processes	JW; ULKR; KVG		VKB; HEMRA; MANDE; JP; SHEIN; ROLRI; INROS; MQUN; *ROHA*; *ASTP*		
3: Fermentation technology	KVG; ULKR; JW	XFA; LRFO; ANLH	LASN; ANB; HILA; ANDNO; *DANAQUH; TIMOH; LMEA*		
Currently active (at the annual meeting)	**3**	**5**	**8**		

1: Research area coordinators are indicated in bold; 2: New PhD-students who have started are indicated in italic, names in italic-parenthesis indicate coworkers who will soon stop; 3: MSc-students who have finished are indicated by italic-parenthesis; 4: External (or visiting) PhD-students who have returned to their home university are indicated by italic-parenthesis. All other names indicate current coworkers at PROCESS.

3.3 Post-Doctoral Research Project Overview

Alberto Quaglia (AQ)

CAPEC
Supervisors: GSI/RaG
Start: 9-2013; End: 2-2014

Design of microbial communities in membrane bioreactors (Ecodesign MBR)

The postdoc project is part of DSF funded center of excellence in "Design of microbial communities in membrane bioreactors" and focus on optimal design and scale-up of a sequential batch reactor (SBR) for autotrophic nitrogen removal. The approach chosen to carry out these tasks lies first on the development of a methodology for bioreactor scale-up. In particular, the following tasks have been included in the research:

- Development of a general framework for model-based scale-up of bioreactors, with special emphasis on mixing operation conditions
- Benchmark of the framework with other commonly used methodologies
- Computer-aided design of optimal design for pilot scale bioreactor
- Quantitative characterization of mixing and shear in the reactor
- Validation with a design proposal for a pilot-scale reactor for autotrophic nitrogen removal

Miguel Mauricio Iglesias (MMMI)

PROCESS/CAPEC
Supervisors: KVG/JKH
Start: 2-2013; End: 7-2014

Modelling and control in industrial solvent recovery units

In the industrial project BIOPRO we are studying, through a model based approach, optimized configurations for multicomponent distillation. The project is articulated on two main topics: modelling multicomponent distillation focusing on the fate of trace compounds (1-10 ppm) and the reduction of the specific energy consumption.
Modelling trace compounds in distillation columns have to rely on a sound thermodynamic description of the vapour-liquid equilibrium. In effect, despite of the relative volatility of the pure compound with respect to the heavy and light key, the activity coefficient can be very high at trace level leading to unexpected behaviour.
In the reduction of the specific energy consumption, we explore integral alternatives (change in control objective, use of heat pumps, mechanical vapour recompression) with different degrees of complexity: from retrofitting solutions that can be applied almost immediately to new designs in the process configuration. Since solvent recovery units are downstream processes that bear the disturbances created upstream, the suitability of any modification in terms of dynamic performance and control are also considered in order to ensure the desired performance.

Xavier Flores-Alsina (XFA)

PROCESS
Supervisors: KVG/LS
Start: 5-2013; End: 4-2015

New process models to simulate, benchmark and control urban wastewater treatment Systems

The objective of this project is to develop a new set of mathematical models describing some of the new focus areas/challenges that wastewater treatment plants are facing nowadays. These new focus areas/challenges include nutrient recycling & recovery, micropollutant removal and energy recovery & greenhouse gases minimization. The most innovative part of the project will rely on finding new ways to operate these facilities satisfying the new demands by means of developing, implementing and simulating novel (plant-wide) control strategies / operational procedures. In order to avoid unbiased comparisons a new benchmarking procedure will be proposed. This procedure will comprise a pre-defined plant layout, simulation models, influent loads, test procedures and evaluation criteria. Finally, the study will be complemented with a multi-criteria decision module that will rank the different technological solutions taking into account multiple aspects at the same time.

Negar Sadegh (NES)

PROCESS
Supervisors: KVG
Start: 1-2014; End: 12-2014

Modeling heat and mass transfer in industrial ovens used for baking

Heat transfer is an important step in the baking process. In the production of baked goods, heat transfer is coupled with mass transfer (water loss). The baking process is governed by heat and mass transfer phenomena. The aim of this project is to develop a better understanding of the baking process in terms of heat and mass transfer to yield improvements in product quality and energy efficiency. The objective of this study is to the enhance energy efficiency of the baking process for an industrial application. The focus of the work is to optimize the performance of the oven chamber used for baking the products. That will be accomplished by developing a robust mathematical model of heat and mass transfer in the baking oven. The oven is a convection oven where the product is heated with hot air. The air flow pattern, the air velocity and the design parameters are important factors for optimizing the performance of the oven.

Nina M. Andersen (nman)

PROCESS
Supervisors: KVG
Start: 5-2014

Modeling and optimisation of an industrial filtration process

Filtration is an important separation step for the company CP Kelco. In this project, an industrial scale filtration operation will be modelled, and the model will afterwards be used to investigate alternative operating strategies for the filtration process, all with the aim of reducing operating costs.

3.4 PhD-Research Project Overview

Rohana Abu (roha)

PROCESS
Supervisors: JW
Start: 10-2013; End: 9-2016

Design and Evaluation for Multi-enzyme Processes

Biocatalysis is attracting significant attention from both academic and industrial scientists due to its excellent capability to catalyse exquisitely selective reactions. Currently, the use of multi-enzyme cascade reaction exhibits excellent advantages over the single step reaction. The benefit could provide the results to organic synthesis problems to produce more complex compounds, especially as pharmaceutical intermediates and provide more efficient reactions compared to single-step conversion. The objective of this study is to evaluate the multi-enzyme system for the process intensification where the engineering tools such as, thermodynamic and kinetic modelling, sensitivity and uncertainty analysis are used to assist the process development. In order to achieve the objective, several case studies of industrial interest are used to evaluate the effectiveness of the systematic approach and to highlight the applicability of the multi-enzyme system for industrial purposes.

Amata Anantpinijwatna (amatana)

CAPEC
Supervisors: RaG
Start: 8-2013; End: 7-2016

Generic model-based tailor-madedesign and analysis of biphasic reaction systems

Biphasic reaction systems contain two immiscible liquid phases such as aqueous/organic, ammonium/organic, supercritical-CO_2/ionic liquid, or two liquid membrane-separated phases. In these systems, reactants and catalyst (including also biocatalysts and enzymes) can exist in different liquid phases, allowing novel synthesis paths as well as higher selectivity, conversion, and yield. Furthermore, after the reaction, reactants, catalyst and products may end up in different liquid phases, making the separation tasks easier. Modelling can be a valuable tool to help with efficient analysis, design, and development of these biphasic reaction systems. However, mathematical models that collectively describe chemical and physical equilibrium, reaction kinetics, and unit operations have not been fully addressed in the open literature. The objectives of this project are (i) to propose a framework for modelling of biphasic reaction systems; (ii) to develop a generic model for biphasic reaction systems from which all other models can be generated; (iii) to apply the framework and the model for designing, optimizing, and analysing the systems of industrial importance.

Marie T. Andersson (mande)

PROCESS
Supervisors: JW
Start: 2-2012; End: 1-2015

Bioprocess Engineering for the Application of P450s

This PhD project is a part of the European research program P4FIFTY and aims for development of process technology and process evaluation tools for biocatalytic cytochrome P450 monooxygenase (P450 or CYP) catalyzed reactions. P450s is a very interesting group of enzymes found in all kingdoms performing specific hydroxylation. The involvement of P450s in drug metabolism in the human liver makes them interesting to the pharmaceutical industry. Furthermore, the difficulties related to the conventional chemical synthesis also make them interesting in the field of white biotechnology. Due to the many challenges this system is facing, the limiting parameter is important to identify for a potential process in order to improve the bottleneck. The PhD project will also handle the need for sufficient oxygen supply as well as suitable reaction media and evaluate oxygen supply methods and solvent systems. In order to optimize the oxygen supply reactor design will be an important aspect and in this work e.g. bubble free aeration will be evaluated.

Deenesh K. Babi (dkbabi)

CAPEC-PROCESS
Supervisors: RaG/JW
Start: 1/8-2012; End: 30-7-2015

Development of a phenomena based approachfor process intensification

Process intensification (PI) is a means by which process industries can achieve a more efficient and sustainable chemical process through the improvement of for example energy efficiency and waste generation. The objective of this project is the further development of the phenomena based process synthesis and design methodology and extension of its application to entire processes together with the development of a computer framework and computer-aided tool for application of the methodology. The algorithm is part of a larger PI framework which is being developed as collaboration between the laboratory of Fluid Separations (FVT), TU-Dortmund and CAPEC, DTU. This framework will allow the intensification of processes through the combination of an experimental and model-based approach.

Research areas: B, C, E

Thomas Bisgaard (thbis)

CAPEC
Supervisors: JA/JKH/NVS/KP
Start: 9-2012; End: 2-2016

Operation and design of diabatic separation processes

Diabatic distillation columns have been proposed as a means to reduce utility consumption and operation cost of separation. In diabatic operation, the heat required to perform the separation is added and/or removed throughout the column. An example is the heat-integrated distillation column (HIDiC), where internal heat transfer is realized by operating the rectifying section at higher pressure than the stripping section, using vapor recompression. The aim of this project is to benchmark diabatic distillation columns against industrially proven configurations, covering the conventional and the mechanical vapor recompression column (MVRC), w.r.t. energy efficient, economics and operation. The benchmarking will include both economical and operational aspects. Status in the project is, that a model framework has been developed, which enables static and dynamic simulations of conventional and heat-integrated distillation columns (e.g. the HIDiC and the MVRC), and a handful of preliminary benchmark studies have been carried out.

Research Areas: B, C, F

Riccardo Boiocchi (ricco)

CAPEC-PROCESS
Supervisors: GSI/KVG
Start: 10-2013; End: 9-2016

Plantwide modelling and control for N2O from WWTP

The project has the primary objective of developing qualified control scenarios directly aiming at the minimization of N2O emissions. The environment in which these control strategies will be developed is given by an extension of the Benchmark Simulation Model no 2. In particular, the simulation model will be first extended in terms of layout and of mathematical model describing the biological processes. Afterwards, model-based and process-insight-based control strategies will be developed. According to a multi-criteria performance evaluation the different control strategies will be ranked and then tested in different plant configurations.

Research area: B,C, E

Hande Bozkurt (hboz)  **CAPEC-PROCESS** Supervisors: GSI/KVG Start: 12-2011; End: 12-2014	***Computer-aided framework for synthesis, design and retrofit of future wastewater treatment systems*** Currently, the WWTP layout designs are mainly based on expert decisions and experiences. This approach takes the values like environmental issues, water reuse, by-product recovery and public impacts into account and identifies the alternatives based on experience, similar solutions and brainstorming to come up with the most viable WWTP systems. However, with increased complexity of the technologies and stricter limit values for effluents; making the most feasible decision with this approach became harder. What is proposed in this paper is therefore, a new approach based on mathematical programming to manage the complexity of the problem and generate/identify novel and optimal WWTP layouts for specific wastewater feed domestic as well as industrial nature. The tool will be developed to formulate the design problem as an MINLP and by using the database of wastewater treatment technologies; it will generate many alternatives and evaluate at their optimality. Since the tool will cover both environmental and sustainability metrics, it will be a powerful decision making agent for WWTP layout design. *Research area: B,C, E*
Peam Cheali (pche)  **CAPEC** Supervisors: GSI, KVG Start: 05-2012; End: 05-2015	***Integrated framework for synthesis and design of multi-product biorefinery networks*** In this PhD project, a framework for synthesis and design of integrated-intensified chemical and biochemical processes is to be developed. This approach allows generation and comparison of a large number of alternatives at their optimal point, in order to identify the optimal raw material, multi-product portfolio and process technology selection for the different cases defined by market scenario, their sustainability metrics and risk of investment under market uncertainties. More specifically, the framework will include the following features: library of models and database for the assessment of process performance, generation and analysis of processing technology alternatives, computer-aided synthesis and design of processing paths in networks, MINLP, assessment and comparison of the candidates at their optimality. Case studies of biorefinery network are considered by focusing on production of biochemicals, biofuels and optimal blends of mixtures with fossil fuels. *Research area: B, C, E*

Larissa P Cunico (lacu)

CAPEC
Supervisors: RaG, Prof R. Cerriani, Dr. B Sarup
Start: 1-3-2012; End: 28-2-2015

Modelling of phase equilibria and related properties of mixtures involving lipids

The objective of this project is to perform a systematic numerical analysis to determine the needs of phase equilibria and related properties in the production of edible oils, biodiesel and other oleochemicals. The available data in literature will be analyzed for consistency and then used to develop/adopt the most appropriate models, for example, group-contribution combined with atom connectivity based models. For systems that are not in literature, some experimental work will be conducted in UNICAMP – Department of Chemical Engineering in Brazil, where the necessary facilities exist. These developed predictive models will be used to determine the sensitivity of design variables with respect to uncertainties in the predicted properties. The application of the developed properties models will be illustrated through case studies involving different lipid compound processing steps. Then, the obtained results will be implemented in process simulation software and will be applied on industrial cases from Alfa Laval Copenhagen A/S as one of the means to validate the models.

Research areas: A, F

Maria Gundersen Deslauriers (mgun)

PROCESS
Supervisors: JW

Enzymatically Assisted CO_2 Removal from Flue-Gas

It is well established that greenhouse gasses are a major contributor towards climate change. About 40% of CO_2 from fossil fuel related emissions originate from coal-fired power plants. The leading technology for CO_2 removal from flue-gas is amine scrubbing. Where amine solvents with a high capture capacity are used to remove CO_2 from the gas. The highly loaded solvent is then transferred to a desorption unit, where the CO_2 is removed by heating. A limitation of this technology is the solvents used. They have several unfavorable properties: solvent degradation evaporation loss and corrosion. Especially high temperatures required in the desorption step is problematic in this setting, because of the large carbon footprint, the very issue this technology is aiming to solve. In collaboration with Novozymes A/S, we are aiming to use enzymes to enhance carbon capture, where solvents with a slow absorption rate will be assisted by enzyme technology, for faster and higher CO_2 capture.

Marina Fedorova (mfad)

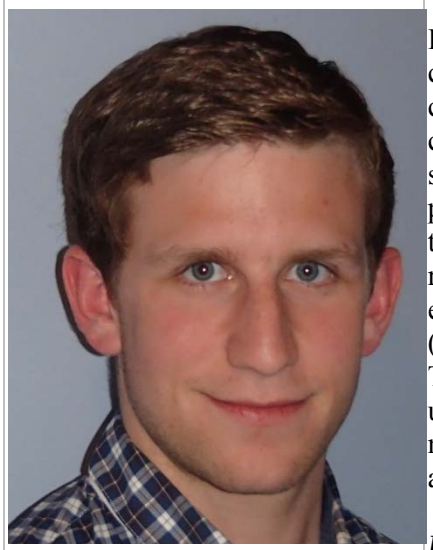
CAPEC
Supervisors: RaG, GSI
Start: 1-4-2012; End: 31-3-2015

Systematic methods and tools for computer aided modelling

Models play an important role of increasing importance in design and analysis of chemicals/bio-chemicals based products and the processes that manufacture them because of the increasing use of computer-aided methods and tools. The advantage of using these model-based methods and tools is that they have the potential to reduce the number of experiments, which can be expensive and time consuming. As the required models may be complex and require multiple time and/or lengths scales, their development and application for product-process design is not trivial. Therefore, the modelling framework can contribute by reducing the time and resources needed for model development and application, thereby reducing the overall time and cost for product-process development. The objective of this project is to develop methods and tools that will allow systematic development of models and their solution using a modelling framework, which consists of a model generation tool, a model analysis-solution tool and templates for solving different modelling problems. Through a number of modelling case studies, the novel features of the modelling framework will be illustrated.

Research areas: B, E, F

Jérôme Frutiger (jfru)



CAPEC
Supervisors: GSI, JA
Start: 6-2014; End: 5-2017

Computer-aided molecular design of novel working fluids to optimize heat transfer processes

In this PhD project which is part of Thermocyc project coordinated by DTU Mechanical Engineering, we will study the characteristics of working fluids and derive novel designs of critical components based on development of application-specific working fluids for the targets specified by the heat pump application. The selection of a suitable working fluid for thermodynamic cycles is important and has to satisfy many requirements ranging from heat transfer ability to safety and environmental constraints such as ozone depletion potential (ODP) and Global Warming Potential (QWP) among others. The fluids must also be chemically stable at any conditions of use, meaning no reaction/oxidation to form by-products, and need to be efficient and compatible with compressor lubricants and equipment materials.

Research areas: B, E, F

Carina Loureiro da Costa Lira Gargalo (carlour)

CAPEC
Supervisors: GSI
Start: 11-2013; End: 11-2016

Sustainable design of biorefinery systems for biorenewables

The sustainable design of a biorefinery system aims to achieve lower water, energy and raw material consumption than the petrochemical refinery producing the same chemical or range of chemicals using fossil-fuels as feedstock. Consequently, a major challenge is to develop the ability to sustainably convert different biorenewables into different value-added products as efficiently as the current petrochemical industry.
The objective of the present project is to propose a systematic multi-level framework which uses superstructure optimization to obtain a base-case design subject to design constraints and a set of performance criteria. The base-case design will be evaluated through sustainability analysis in order to logically identify the process hot spots. The obtained information is then used to set design targets for achieving a more sustainable design through retrofitting techniques.
In order to validate the framework, it will be applied to generate the superstructures of lignocellulosic and vegetable oil biorefinery to biofuels and bioproducts, and identify the respective optimal solutions with respect to the selected set of constraints.

Research area: B, C, E

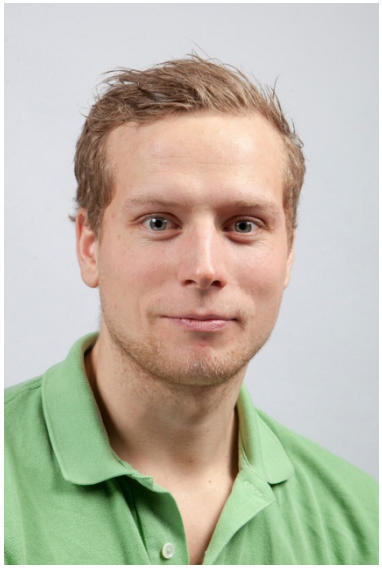
Zainatul Bahiyah Binti Handani (zbha)

CAPEC
Supervisors: RaG, GSI
Start: 5-2013; End: 4-2016

Integrated synthesis and design of chemical processes and waste water treatment neworks

Increasing of social awareness of the importance of water conservation and the escalating costs of freshwater and effluent treatment are pushing process industries as well as the modern society to develop more efficient and effective ways to manage their water balance. In this project, a generic model-based framework for the optimization of water and wastewater networks integrated with their associated chemical or biochemical processes will be developed for the benefit of the modern society and more specifically, for process industries by reducing the consumption of freshwater and re-using more processed water as well as obtaining a more sustainable overall process design. The synthesis problem will be formulated as Mixed Integer Non Linear Programming (MINLP) and different variations of it. First principles modelling coupled with data-based modelling will be used to develop a library of models representing all operations in water networks.

Research area: B, C, E

Søren Heintz (shein)  **PROCESS** Supervisors: KVG, JW, ULKR, PT BIOINTENSE EU-funded 7th Framework project	***Mastering Process Intensification across Scales for ω-Transaminase Processes*** This project takes its focus on the development of miniaturized platforms and toolboxes, which provide novel means to achieve fast screening of new processes, thereby resulting in a reduction of the process development time. A main driving force for developing the miniaturized platforms is the reduced quantity of expensive and/or scarce resources needed for evaluation of potentially promising process candidates at micro-scale. In addition, miniaturized reactors allow real time monitoring (have to undergo further development) and better control, as well as improved safety of the process. The development of the platforms and toolboxes in this project will be based on case studies with ω-transaminase facilitated processes. The challenges with these transaminase processes are, for example, general unfavorable reaction equilibriums and inhibition from substrates and products. Some of these challenges are intended to be overcome by setting up different process operation strategies, for example, In-Situ Substrate Supply (ISSS), In-Situ co-Product Removal (IScPR), and In-Situ Product Removal (ISPR).
Sawitree Kalakul (sawit)  **CAPEC** Supervisors: RaG, (Georgios Kontogeorgis, Bent Sarup) Start: 6-2013; End: 5-2016	***Property modeling and process design involving complex chemical systems*** Complex chemical systems in this project are defined as liquid mixtures containing combinations of lipids, solvents, inorganic salts and water. Commercial process simulators, which are increasingly used in process design and analysis, usually lack the necessary physical and thermodynamic property data and/or models for many of the lipids in their databases. Multiphase electrolyte system models often have severe limitations in their applicability for the processes mentioned above. This limits a wide application of computer-aided methods and tools for process synthesis, modeling and simulation within edible oil, crude fossil fuel production and related industries. The objective of this project is to evaluate the requirements of the property models together with the available data to determine the property model needs, and based on this, to develop property models on demand for use in design-analysis of processes handling lipids and other chemicals. A second objective of this project is also to apply the developed property models for the tailor-made design of jet-fuels. *Research areas: A, B, C*

Hilde Larsson (hila)

PROCESS
Supervisors: ULKR, KVG, Anne Ladegaard Skov

Modeling and topology optimization of fermentation processes in microbioreactors

The main aim of this project is to improve the productivity and reliability of microbioreactors for fermentation processes, mainly through process modeling and computational fluid dynamics (CFD). Microbioreactors do offer several advantages compared to the use of shake flasks and microtiter plates for purposes such as screening and process optimization, but there is yet no industrial standard in using them. Reactions occurring in microbioreactors can for example more easily be monitored and controlled both offline and online and they also require very little laboratory space and chemicals. Once mass fabricated, microbioreactors can also have a very low cost per unit and they are also disposable which makes them less labor intensive than shake flasks and similar options. But significantly more development is needed for microbioreactors to become a standard in industry and academia, similar to for example microtiterplates. The microbioreactors need to be more reliable and easy to handle and the interpretation of their results needs to be more straight forward aiming at process scale up to pilot or production scale.

Seyed Soheil Mansouri (seso)

CAPEC
Supervisors: RaG, JW, JKH
Start: 9-2013; End: 8-2016

Design, control and analysis of intensified chemical and biochemical processes

The current societal requirements and the state of environment, call for accelerated development of more sophisticated and efficient process systems. Process Intensification (PI) is one of the many options to match current and future challenges of the (bio)chemical industry and it has the potential to improve existing as well as conceptual processes to achieve a more sustainable and economic production. Furthermore, advancements in economic, sustainability and safety of intensified chemical processes can be obtained if control and operation of intensified equipment is considered systematically together with different PI options. Currently there is no generic framework for simultaneous design, control and analysis of intensified processes. Therefore, this project aims at incorporating process synthesis, design, intensification and control into one systematic framework. By application of this proposed framework the intensified design option is designed so it that it has the natural ability to reject disturbances resulting in an optimal and self-regulating design. The intended design is also an optimal design with respect to sustainability and economics.

Program Areas: C, D, E

Michele Mattei (micu)

CAPEC
Supervisors: RaG, GK (AT-CERE)
Start: 8-2011; End: 7-2014

Development of a systematic methodology for emulsion based chemical product design

The goal of chemical product design is to find a product that exhibits a set of desirable or specified behavior. A chemical product design problem can be summarized as follows: given a set of desired (target) properties, establish a list of chemical formulations satisfying these targets and then choose from them the most appropriate candidate to be verified experimentally. The chemical product of interest can be a single chemical or a mixture/blend; a formulated product is a mixture that contains different chemicals, active ingredients as well as additive. The objective of this project is to develop a systematic methodology for the design of emulsified chemical products. The methodology will employ a model-based product synthesis /design stage and a model-experiment based further refinement and/or validation stage. The success of any model-based methodology depends on the availability of reliable and predictive models. The project therefore will also develop, where necessary, the required property prediction models for emulsions. Design of consumer products will be considered as suitable case studies.

Research areas: A, C, F

Kresten T. Meisler (kretm)

CAPEC-PROCESS
Supervisors: RaG, KVG, NVS
Start: 3-2011; End: 9-2014

Multi-dimensional population balance models of crystallization processes

The project aims at describing the complex phenomena occurring during a crystallization operation in multiple dimensions. The phenomena include nucleation, growth, breakage and agglomeration and a population balance model is based on the phenomena allowing calculation of the multi-dimensional crystal size distribution (CSD). The translation of measured data for monitoring of crystallization operations is used for model parameters and the full model with parameters is used for analysis of the crystallization process through simulation within a framework describing the balance equations. With the simulations different operational policies and process options are explored through generation of the CSD for the systems. An operational policy for the desired crystal size distribution for a given crystallization process is designed.

Research area: B, C, D

Aleksandar Mitic (asmi)  **PROCESS** Supervisors: KVG, KDJ (CHEC) Start: 15-11-2010; End: 14-11-2013	***Operational aspects of continuous pharmaceutical production*** Most pharmaceutical productions are based on batch and semi-batch processes and involve many problems, such as long reaction sequences, non-uniform conditions inside vessels, implementation of PAT applications. Continuous manufacturing might offer a solution to those problems. Therefore, the main focus of this PhD project is to develop efficient continuous production of zuclopenthixol, a product of H. Lundbeck A/S. A grignard reaction, hydrolysis and a dehydration reaction should all work in continuous mode with high selectivity in order to avoid intermediate crystallization steps. Simplifications and improvements of the liquid-liquid separation, as well as acceleration of the slow hydroamination reaction are additional challenges. Potential use of micro-scale equipment, such as microreactors and L-L microseparators will be tested. Also, on-line monitoring and control of the established continuous process will be studied. Applications of NIR spectroscopy will be tested.
Ane Loft Mollerup (molle)  **CAPEC** Supervisors: GSI Additional supervisors: Peter S Mikkelsen, Dines Thornberg Start: 8-2011; End: 11-2014	***Optimizing control of the integrated urban wastewater system*** Since the EU Water Framework directive came into force in 2000, wastewater systems (sewer system and wastewater treatment plants) in Europe have been put under pressure to reduce the number of combined sewer overflows (CSOs) from the system to protect the aquatic environment. The aim of this project is to formulate the problem of design and analysis of the regulatory level from a process control perspective and to develop a methodological approach to find the optimal solution. The project aims at developing a methodology for determining the best control structure and technique for an integrated system of both sewer system and wastewater plants, when optimizing towards defined objectives, e.g. minimizing flooding, overflow from the sewer system, bypass from the WWTP, electrical consumption, etc.One of the issues to be examined is the robustness of the control structure with respect to actuator failure and uncertainty on measurements.Also the optimization of the system is addressed. With the introduction of better climate models and radar predictions of the precipitation it might be possible to introduce a supervisory control layer with Real Time Optimization (RTO). *Research area: B, D*

Anders Nørregaard (andno)

PROCESS
Supervisors: KVG, JW, Sturat M. Stocks, Brian Madsen, Frans van den Berg

Mixing and oxygen transfer processes in bioreactors

In this project, computer based models will be used to analyse and predict the performance of fermentation processes. One of the main challenges while creating the models is managing the imperfect mixing in the bioreactor which leads to oxygen and substrate gradients. The fermentation broth is a non-newtonian shear thinning liquid that constantly changes composition and properties during the fermentation process. Modelling the viscosity of the fermentation broth is a challenge as well, since this factor influences mixing efficiency and oxygen transfer significantly. The goal of the project is to identify improvements to the bioreactor design together with improved operating conditions in order to achieve a higher energy efficiency of the process. It is within the scope of the project to test one of these proposed improvements in a production scale bioreactor.

Emmanouil Papadakis (empap)

CAPEC
Supervisors: RaG, GSI, KVG
Start: 10-2013; End: 9-2016

Modeling and Synthesis of Pharmaceutical Processes: Moving From Batch to Continuous Manufacturing

The pharmaceutical industries are dominated by batch wise processes, which have served well the pharmaceutical industries as well as the regulatory bodies. Generally the batch processes are not very efficient for product quality assurance and possess a number of drawbacks such as poor process understanding, low productivity, high energy consumption, high capital cost, low product purity, scalability and waste production. Continuous pharmaceutical manufacturing is an attractive alternative, which naturally eliminates some of the drawbacks of the batch processing while maintaining the flexibility. Methods and tools which have been applied in other industries (such as chemical and petrochemical) for design and operation may not directly be applicable in pharmaceutical processes. The objective of the study is the development of an integrated framework which can facilitate the move from batch towards the continuous pharmaceutical manufacturing by using computer aided methods and tools, and to be applicable in multipurpose production line. The integrated framework is intended as an enabling technology for the development of greener pharmaceutical processes with higher economic feasibility, safer and improved product quality.

Research program areas: B, C, D

Jason Price (japr)  **CAPEC-PROCESS** Supervisors: JW, JKH, MAN Start: 01-09-2011; End: 01-10-2014	***Operation and Control of Enzymatic Biodiesel Production*** This work explores the control of biodiesel production via an enzymatic catalyst. Currently enzymatic catalysts are not in widespread use for commercial-scale biodiesel production. This is mainly due to non-optimized process designs. Furthermore is it unclear what process variables need to be monitored and controlled to ensure optimal economics. Critical to the project is to develop a control methodology to optimize the productivity of biodiesel production. The implementation of a control system to handle changes in the feed composition and the correct dosing of alcohol can potentially lead to very large energy savings and at the same time provide a more consistent product quality. However given most conversion and quality analyses of biodiesel are commonly done by chromatographic methods, suitable measurement techniques will need to be investigated to obtain real-time information on the states of the system. The main deliverable is a steady state and dynamic simulation model of the process including a strategy for monitoring and process control. This model and the proposed strategies will be validated experimentally on the department's pilot facilities. *Research area: B, D*
Daniella Quintanilla (danaquh)  **PROCESS** *Supervisors: KVG*	***Linking Strain Morphology to Rheology and Mass Transfer as a Means to Improve Fermentation Processes*** Manipulation of media, strain improvements and various parameter optimizations are among the most relevant strategies for promoting the overproduction of bulk enzymes in fermentation processes. However, further improvements are needed if enzyme cost has to be reduced to make some processes economically feasible. Filamentous microorganisms are widely used as hosts in the production of these enzymes due to their ability of secreting large amount of proteins, post-transcriptional modification machinery and the fact that a large number of species are generally recognized as safe. Nevertheless, they also present major disadvantages, due to the unavoidable oxygen transfer limitations as a consequence of the high viscosity of the medium that they develop, which is believed to be related to the biomass concentration, growth rate and morphology. These will be fully studied in this project, since morphology is believed to be linked to the process productivity at the microscopic and macroscopic level. Therefore as well, fungal morphology is usually a bottleneck for productivity in industrial production. This will allow us to determine whether a certain microorganism's phenotype has an influence on process performance, and how this performance can be influenced actively by manipulating different process variables or by genetic engineering of the strain, as a means of improving the design and operation of filamentous fungal fermentations.

Rolf Hoffmeyer Ringborg (rolri)

PROCESS
Supervisors: JW, KVG, ULKR

µ-Tools for Development of ω-Transaminase Processes

The focus of this thesis is to develop µ-technology and toolboxes that can be used for feasibility screening of new processes. The development will focus on the enzyme ω-transaminase (ω-TA), this catalyst has shown challenging difficulties in relation to thermodynamics and economic feasibility. The motivation for this enzyme is the prospect of being able to asymmetrically produce chiral amines. Chiral amines occur in many API's and hence require very high purity. Obtaining optically pure chiral amines are highly desired as they will reduce side effects of the unwanted enantiomer and yield a higher product quality. This will also pass FDA legislation that requires a 99% enantiomeric excess.

BIOINTENSE EU-funded 7th Framework project

Ines Periera Rosinha (inros)

PROCESS
Supervisors: ULKR, JW, KVG, Anders Daugaard

Topology optimization in biocatalytic reactions using miniaturized

This project will focus on the development of microbioreactor configurations and the optimization of the spatial distribution of immobilized enzymes in order to overcome this limitation. The strategy to select the reactor will be different from what is usually done. Instead of adapting the process to a well-known reactor shape, a topology optimization method will be used to find the reactor shape with best performance. This reactor will be fabricated and tested in laboratory. This project has also the aim to investigate whether the spatial distribution of immobilized enzymes on the reactor surface can contribute significantly to improve reactor performance.
This project will focus on an integrated approach of model based and experimental investigation of the best microbioreactor configuration for supporting immobilized ω-transaminases. With the help of structured kinetic models, Computational Fluid Dynamic (CFD) models and fabrication of miniaturized reactors in different materials, several parameters will be studied and optimized.

Catarina Sanches Seita (casse)

PROCESS
Supervisors: JW

Bioprocess evaluation tools

During the last few years considerable progress has been made in the production of organic compounds by means of fermentation or biocatalysis. Bioprocesses based on these biocatalysts have emerged as an alternative to conventional chemical synthesis driven by the need for selective synthetic routes, with high reaction yield and few side reactions, as well as the use of renewable and biodegradable raw materials and catalysts and the fact that biocatalytic reactions run under mild conditions in aqueous solutions. All these features make bioprocesses as alternatives with great potential for "green" and selective processes and its application is steadily increasing at an industrial scale. However, since it is a relatively new technology and given the complexity of the development process, many bioprocesses do not fulfill the economic requirements for industrial operation (high reaction yield, high biocatalyst yield, high product concentration and high space-time yield). This project aims to develop a range of adequate tools to evaluate bioprocesses in different development stages from three different perspectives – technical, economic and environmental.

Laura Snip (lasn)

PROCESS
Supervisors: KVG

Practical Application of Models in the Urban Water System: Simulation Based Scenario Analysis

With the increasing awareness of global warming also wastewater treatment plants (WWTPs) have to monitor their production of greenhouse gases (GHGs). Besides GHG emissions, a WWTP has a relatively new challenge as well. Indeed, with the development of methods to measure chemicals at low concentrations, a growing awareness of the presence of micropollutants in the aquatic environment has been established. WWTPs are traditionally not designed to remove micropollutants, but a change in operational conditions can increase the removal of micropollutants in a WWTP.
The Benchmark Simulation Model 2 (BSM2) will be extended in this PhD study to include the processes concerning GHGs and micropollutants. Once this extension is made the model will be calibrated and validated with data from full scale wastewater treatment plants. After the calibration and validation, different scenarios will be compared according to newly developed evaluation tools. These evaluation tools should also include criteria concerning GHG emissions and micropollutants besides the current effluent quality index and operational cost index. Also, different control strategies will be tested to investigate potential improvements of plant operation.

Anjan Kumar Tula (antu)

CAPEC
Supervisors: RaG, GSI
Start: 12-2013; End: 12-2016

Computer Aided Methodology for Process Flowsheet Generation, Design & Analysis

Process synthesis involves the identification of the optimal path to reach a desired product from a given starting point, of the desired quality and quantity, and subject to defined constraints on the process. In general, existing methodologies for process synthesis can be classified into three main classes: (1) Heuristics or knowledge based methods; (2) Mathematical or optimization techniques; (3) Hybrid methods, which uses knowledge from the previous two methods. So there is a need for systematic process synthesis framework to produce reliable and more consistent designs faster. Therefore this project aims at developing such a framework, which relies on the combined use of systematic methods for flowhseet generation, selection and design for obtaining sustainable designs in shorter synthesis cycles. The methodology to be used to generate all possible process alternatives will be a hybrid approach which incorporates both the physical insights of the knowledge based methods with mathematical programming techniques to formulate and solve a superstructure based optimization problem. Based on the framework, integrated tool will be developed and its application will be highlighted through case studies.

Research Programs: B, C, E

Andreas Åberg (aben)

CAPEC
Supervisors: JA, JKH
Start: 8-2013; End: 7-2016

Modeling and Operation of Diesel Engine Exhaust Gas Cleaning Systems

The focus of this project is to develop a methodology to model and control transient systems. The application used to develop the metodology is the automotive SCR catalyst for heavy duty diesel engines. The SCR catalyst removes nitrogen oxides from the exhaust gases, which are a main contributor to smog in urban areas. This is done by injecting urea before the catalyst, which decomposes into ammonia. The ammonia is used in the catalytic reactions. The challenge with this system is that it in practice never reaches steady state, and it is therefore a challenging control problem to dose the correct amount of urea to the catalyst. The project is in close collaboration with Haldor Topsoe A/S.

3.4 External PhD-students (projects)

Pichayapan Kongpanna
Chulalongkorn Univ., Thailand (s132070)

CAPEC
Supervisors: RaG
Start: 8-2013; End: 7-2014

Design and analysis of CO2 utilization based chemical and biochemical processes

Carbon dioxide accumulation in the atmosphere is a major cause of increasing global temperature and severe climate changes. The CO_2 utilization has become an interesting topic especially with respect to conversion of CO_2 to valuable chemicals. A systematic superstructure-based methodology is developed for design-analysis of CO_2 utilization processes. Sources of Co2 emmission are identified, the conditions under which the CO2 could be utilized as a reactant in the production of useful value-added products obtained through database search, and a superstructure of all possible process paths is generated. The optimal network, which is a collection of processing steps having at least one step where CO2 utilization is involved, is then determined by solving optimization problem. The network is analyzed in terms of economic, sustainability and life cycle assessment criteria in addition to process operability and product specification. The final result is a more sustainable design of a process utilizing captured CO2, producing a useful value-added product. One of the criteria for acceptance is that the more sustainable design alternative must show a net reduction of CO2 emmission. The methid has been applied to the design of a dimethyl carbonate process utilizing captured CO2.

Main supervisor at Chulalongkorn University: Prof Suttichai Assambumrat

Kosan Roh
KAIST, South Korea (kosroh)

CAPEC
Supervisors: RaG
Start: 5-2014; End: 11-2014

Superstructure based-techno-economic feasibility study of thermochemical CO_2 conversion technologies for methanol production

The objective of this project is to study the techno-economic feasibility of various immature CO_2 conversion technologies via the superstructure model-based approach. It aims to perform the preliminary analysis for CO_2 conversion rather than capture and sequestration. Four different kinds of reforming reactions (Tri-reforming, bi-reforming, dry-reforming, and partial-oxidation) and methanol synthesis reaction, relatively well-developed thermochemical CO_2 conversion technologies, are within the scope of our research. We develop a superstructure model containing all possible technical options of four reforming reactions and methanol synthesis via the literature survey, and find the optimal processing pathway by solving MINLP optimization problem with the objective functions of maximum CO_2 utilization or minimum operating cost. Also, sensitivity analysis is performed to study the effects of various techno-economic parameters on the selection of the optimal pathway.

4. CAPEC Software

Development of CAPEC software is closely related to the CAPEC research projects. Since a majority of CAPEC research projects deal with the use of computers to solve process/product engineering problems, the theories and algorithms developed in the research projects are validated through these computer programs. Among these, the computer programs that have a general appeal with respect to their application and do not have any restrictions imposed by a consortium member company, are collected and distributed as part of the CAPEC software. CAPEC software is not a commercial software and are distributed exclusively only to the CAPEC industrial consortium member companies. A special version is distributed at a nominal price for educational purposes.

The objective of the CAPEC software is to promote the use of computer aided methods and tools developed by CAPEC in the solution of current and future process/product engineering problems. The CAPEC software consists of the following:

- Integrated Computer Aided System – ICAS
- EXCEL based macros (ProPred, CAPECDB Manager)
- UNIFAC-Utility (group definitions, VLE database, etc.)
- Special Software (ICAS-PAT, SustainPro, *v*PPD-*Lab*, ECON, LCSoft, AzeoPro)
- PC-SAFT software package
- SMSWIN – A tool for properties and phase equilibrium calculations, especially suitable for solid-liquid systems (compliments with the features in ICAS)

4.1 Integrated Computer Aided System – ICAS 17.0

ICAS combines computer-aided tools for modelling, simulation (including property prediction), synthesis/design, control and analysis into a single integrated system. These tools are present in ICAS as toolboxes. During the solution of a problem, the user may move from one toolbox to another to solve problems requiring more than one tool. For example, in process synthesis, one option is to define the feed stream, then analyse the mixture (analysis and utility toolbox), then generate a flowsheet (synthesis toolbox), then optimise the flowsheet (design toolbox), and finally verify the design (analysis toolbox). From any toolbox it is possible to invoke the simulation engine to perform steady state and/or dynamic simulation for batch and/or continuous process operations. From the synthesis toolbox, it is possible to invoke the solvent design tool (in design toolbox) if a solvent is needed for a specific separation task. There is also a utility toolbox, which determines properties, phase diagrams, etc., which can be used by the other toolboxes or by the user to analyze the behaviour of the specified system. “ICAS documentations” provides information on installation of ICAS, tutorials at basic and advanced levels and other useful information such as a list of dll-files copied during installation and new features of the latest version of ICAS. Figure 4.1 highlights the idea of integration and the advantages that can be obtained through this integration.

In ICAS 17.0, new features have been added to the following tools: ProPred (pure component property prediction), MoT (modelling toolbox), ProCamd (computer aided molecular design), and SolventPro. In addition, bug fixes and improvements have been made in ProCAMD and the CAPEC-database. A new tool, AzeoPro, has been added to ICAS. The EXCEL based macros (ProPred and CAPECDB manager) have been updated with new features and corresponding manuals. The CAPECDB manager also includes an azeotropic data collection and analysis feature. In addition, three special software (EXCEL based): Sustain-Pro, ICAS-PAT, ECON and the Virtual PPD-lab (*v*PPDL) have been revised and improved. Also, LCSoft has a new and improved version. Each of these software, use a number of ICAS tools and models generated through MoT. For a list of ICAS tools, see ICAS Documentation or the ICAS poster. A number of new properties for organic chemicals as well as polymer repeat units have been added to ProPred. ProCAMD, ProPred, Database have been integrated through SolventPro.

ICAS: combines computer-aided tools for modelling, simulation, property prediction, synthesis/design, control and analysis into a single integrated system

- **ICAS** is dedicated to manage the complexity through a systems approach
- **ICAS** algoris are based on a systematic solution approach
- **ICAS** allows single- and multi-dimensional problems to be solved efficiently, reliably, consistently and robustly
- **ICAS** improves productivity by allowing sharing of common knowledge between different groups of people

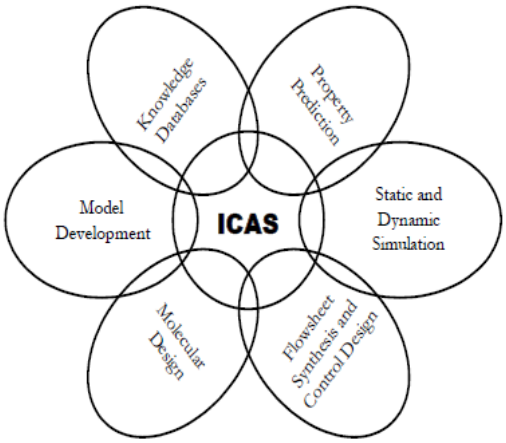


Figure 4.1: The idea of integration within **ICAS**

In general, **ICAS 16.0** has become a much more robust and reliable version of ICAS with a wider application range. New additions to ICAS are also highlighted in the corresponding ICAS-tools manuals. New versions of manuals for the following tools in ICAS are also available - ProPred, MoT, ProCamd and SolventPro. After installation of ICAS, users will find a number of worked out examples given in the "examples" and "tutorials" directories. Figure 4.2 highlights the new features in **ICAS 16.0** while Fig. 4.3 highlights the work-flow in the implementation of a model (starting from transferring the published model equations to MoT and ending with a COM-object that can be executed from different external software).

ICAS-Tools

Database Manager

ProCAMD

ProPred

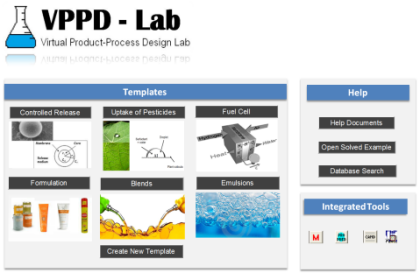
MoT & TemMod

SolventPro

SolventPro
Solvent Selection tool

New Software

VPPD-lab (new version)



New features include blend (gasoline, lubricant) design and emulsified formulations

Other-Tools

SustainPro
Sustainable process design

LCSoft
Life cycle analysis

ECON
Economic analysis

ICAS-PAT
PAT system design

Azeopro
Separation of azeotropic mixtures

Figure 4.2: Highlight of new features in ICAS 17.0

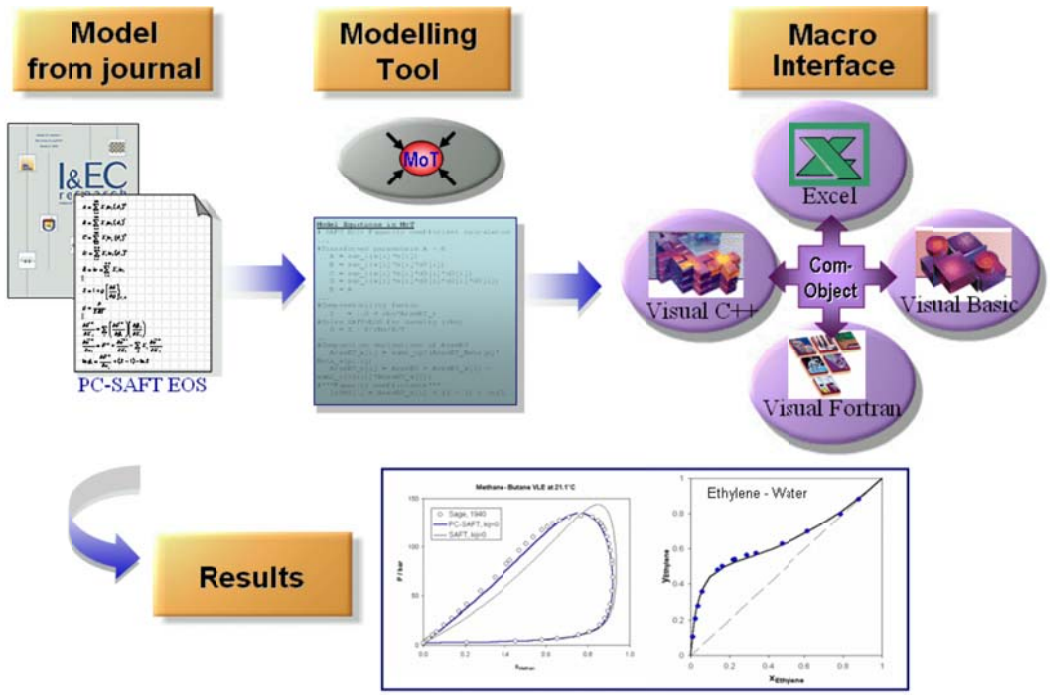
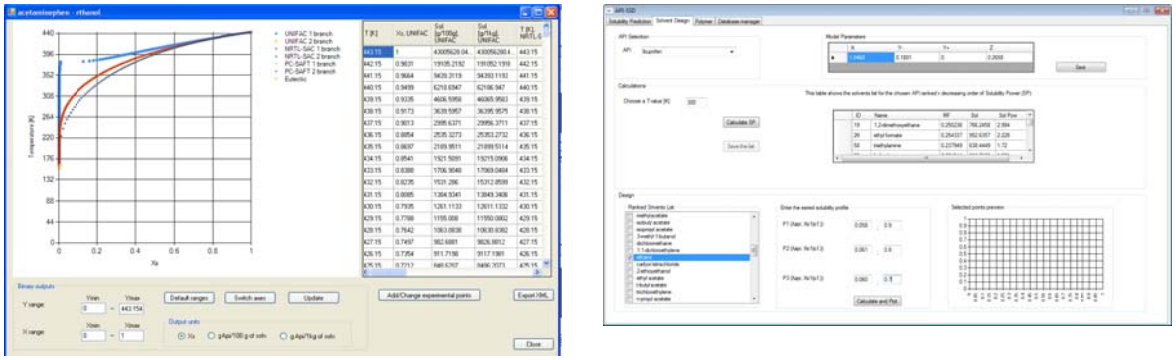


Figure 4.3: COM-object generation through MoT and use in external software

In ICAS 17.0, MoT has new features (see the MoT new features document); ProCamd and SolventPro have had bug-fixes; a new solvents database has been added to the CAPECDB (EXCEL version); and SustainPro and the LCSoft have new versions.

In ICAS 17.0, Propred 4.4 has a number of new additions and updates. These new features includes revised estimations of 10 environment-related properties (LC50,GWP, …) of organic compounds using MG method with uncertainty estimates, estimation of lipids properties including single and temperature dependent properties by MG method, an extended internal database (with more than 23000 molecules), revised and improved property estimation (heat of formation and enthalpy of fusion), estimation of new properties such as liquid thermal conductivity, user friendly navigation features, quantification of prediction uncertainties (95% CI). In SolventPro, a feature for calculation and analysis of solid solubility has been added (see Fig 4.4).



(a) (b)

Figure 4.4: New features of SolventPro. Solid solubility (4.4a); solvent selection (4.4b)

4.2 EXCEL based macros for ICAS-tools (ProPred, CAPECDB Manager)

Two EXCEL based software have been further improved to facilitate the use of ICAS-ProPred and the CAPEC-database:

- EXCEL-ProPred, the user opens the EXCEL macro and then performs different property calculations through ProPred. Here, the EXCEL spreadsheets become the working area and ProPred is the property calculator.
- In the CAPECDB Manager, the EXCEL macro helps the user in the search for data available in the CAPEC database. A new feature to this database is the availability of azeotropic data. A solvents database consisting of information on approximately 1400 solvents has been added.

4.3 UNIFAC-Utility

KT-UNIFAC-utility is a program that helps the user to check the consistency of UNIFAC groups, their parameter values and the representation of the molecules with the UNIFAC groups. For a specified mixture, the program determines the UNIFAC group information and passes the relevant data to ICAS for use in TML and other tools.

4.4 EXCEL-based integrated software (ICAS-PAT, SustainPro, vPPD-lab, ECON, LCSoft)

ICAS-PAT

ICAS-PAT is an EXCEL based software that designs and/or analyzes a process monitoring system, given the process information. It has a built-in knowledge base of information about process operations, the variables that need to be measured, the variables that need to be monitored and the equipments that could be used. It also has a library of models that may be needed to supplement the data available for the process under investigation. The library models are run through ICAS-MoT. The EXCEL macro guides the user through an established work-flow based on the systematic methodology developed by Singh et al. (see PEC08-05). A manual and several solved case studies are available. New features include models for crystallization operations. Figure 4.5a highlights the main features of ICAS-PAT.

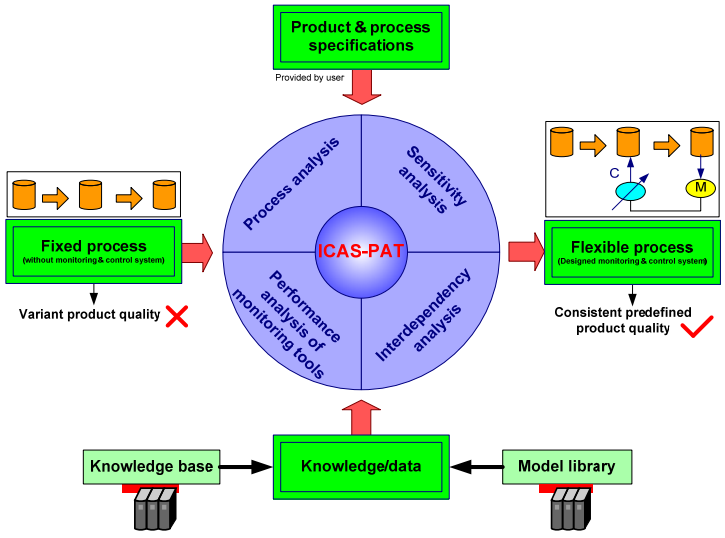


Figure 4.5a: Overview of the main features of ICAS-PAT.

SustainPro

SustainPro is an EXCEL based software, which provides options for retrofit analysis and performance analysis of a given process. A new version is now available with more automated steps and a number of worked out examples. The objective is to perform sustainable process design through SustainPro (see also PEC12-55).

The inputs to *SustainPro* are the mass and the energy balance data that can be collected either from the plant or from process simulations. To perform the retrofit analysis, *SustainPro* also requires as

input, several cost related data (the prices for utilities, the prices for chemicals, etc.). *SustainPro* is able to read the mass and the energy balance from an EXCEL file generated by a commercial simulator. The EXCEL interface guides the user through the steps of the work-flow (solution steps). After applying all the steps *SustainPro* gives as output for the retrofit analysis, a new design alternative suggestion for improving the process being investigated. When the software is used for performance analysis, the output provides the calculated values of the sustainability metrics and the safety indices. After applying the retrofit analysis, the performance analysis is performed and compared with the base case design.

LCSoft

The present framework includes LCSoft software that systematically calculates the important LCA factors (PEC14-18). LCSoft is employed to estimate the carbon footprint and the potential environmental impacts (PEI's). Figure 4.5 shows the Main user's interface of LCSoft.

As input data, the software needs a detailed mass balance of the production process and the duties of all equipment in the process. Additionally, a careful analysis on the system boundaries must be performed since one needs to specify the origin of each compound present in the system. In other words, one needs to know the origin of every compound that is shown in the mass balance, whether it is a product, by-product, chemical or raw material. Figure 4.5 highlights the work-flow related to LCA factor evaluations.

LCSoft

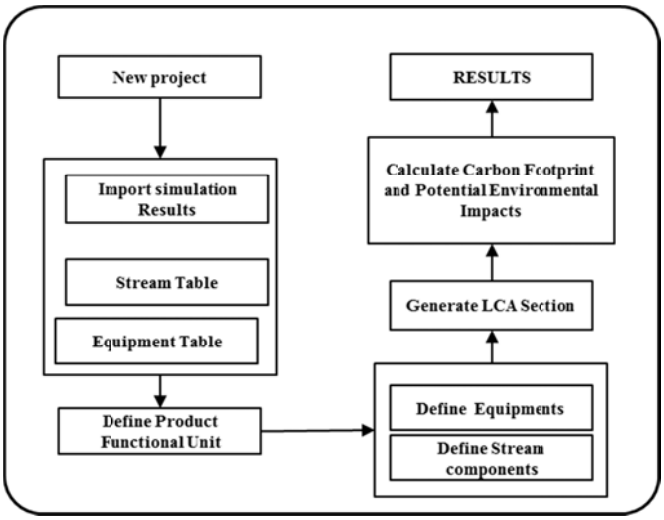


Figure 4.5b: Overview of the main features of SustainPro

Virtual Product-Process Design Lab

The idea behind the virtual product-process design lab is the following: instead of doing the experiments needed to search for a product and its process to manufacture it, the engineer/scientist performs *virtual* experiments, through the *v*PPD-lab software. The software therefore contains a large knowledge base of data (of chemicals, of solvents, of plants, of microcapsule devices, etc.); a large collection of models (models for property prediction, models for controlled release, models for mixing, etc.); of design algorithms (methods for formulation design, methods for molecule design, methods for polymer design, methods for process flowsheet synthesis, etc); other tools (property prediction software; model generation software; equipment design software; design of experiments software, etc.). All of the above are organized through a framework for efficient management of the complexity. Figure 4.4c gives an overview of the main features of the *v*PPD-lab software, which has been used in the design and evaluation of the controlled release of a drug active ingredient (codeine) through a polymeric microcapsule. In the first step the problem is defined (identity of the active ingredient; the desired controlled release parameters, etc., are given in the "documentation" box of *v*PPD-lab). In the second step the selection of the application source (codeine released into the

body), the primary properties of solvent and the polymer (needed by the controlled release model) is made (if the user is unable to provide this information, methods for solvent design and polymer design are used to generate a list of candidates to select from). In the next step the selection and calculation of the functional properties needed to evaluate the controlled release design is made (if models are not available, the modelling software helps to generate new models). In the next steps, the product performance model is used to predict the product behaviour. If the desired (target) performance is matched, then the last step of verifying the product performance through experiments is performed. If the target is not matched, it is possible to repeat from any of the earlier steps with a new design alternative. An option for formulation design together with the associated databases has been added.

Important issues to note from this example are that multi-scale models have been used, data and knowledge from different disciplines have been used and, design/evaluation problem has been effectively used by solving a collection of sub-problems according to a pre-determined sequence. The final step (not shown) would be to select a few of the alternatives and perform the necessary experiments to validate the selection. Therefore, the experiments are done not to design the product but to verify the product. This approach has the potential to save time and money in bringing a chemical based product to the market. Obviously, the accuracy and range of application of the *v*PPD-lab software depends on the available data and models in the software.

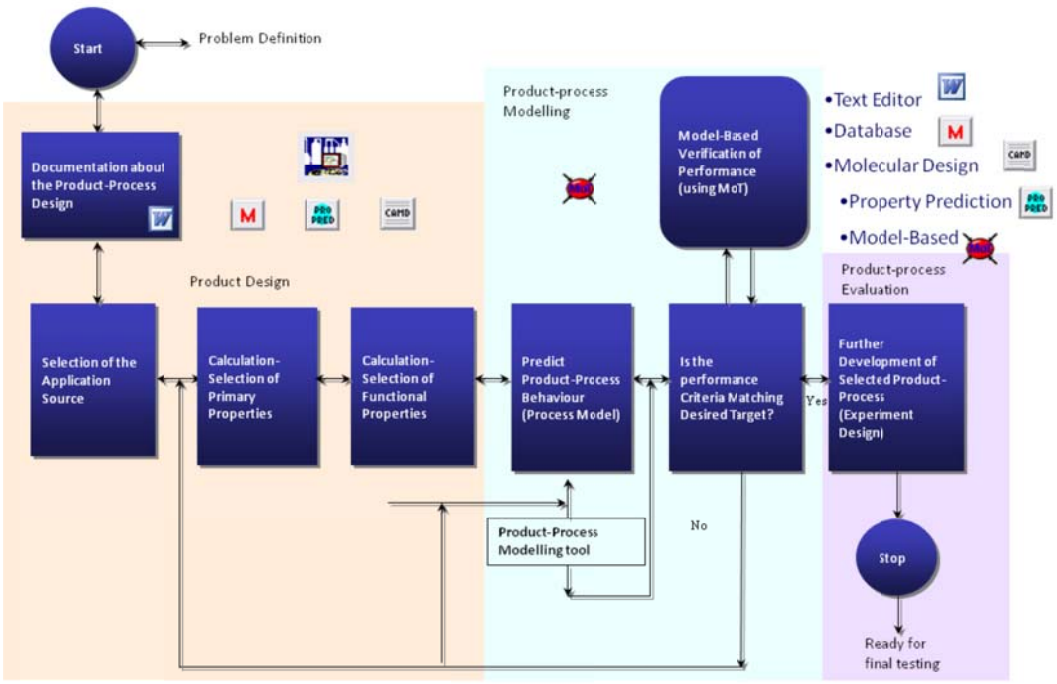


Figure 4.4c: The virtual product-process design lab

4.5 PC-SAFT Software Package

This software performs multicomponent phase equilibrium calculations at given temperature with the PC-SAFT equation of state.

- The user firstly provides some information about the molecules involved in the mixture and gives the molar fraction of each of them. The temperature of the mixture is also required. Molecules may be chosen from an extended databank of nearly 1000 compounds (including some polymers) or may be created from GC^{+} methods.
  Once the mixture completely described, the user chooses between two kinds of calculations:

- **[1]** *bubble point calculation:* The mixture is assumed to be a saturated liquid. The software calculates the bubble pressure and the composition of the vapour phase in equilibrium (a single bubble in this case).
- **[2]** *dew point calculation:* The mixture is assumed to be a saturated vapour. The software calculates the dew pressure and the composition of the liquid phase in equilibrium (a single droplet in this case).

4.6 SMSWIN

SMSWIN is a software package that Syngenta has given to CAPEC for maintenance, further development and integration with ICAS. SMSWIN has a database of compounds and their properties, a collection of property models for phase equilibrium calculations, which are especially suitable for solution properties involving solids. Currently, ProPred and the KT-UNIFAC model have been integrated with SMSWIN.

A new version of SMSWIN is available. The following changes are made in the new version: (i) the default units are now °C and Bara (750mmHg) for all the plots, and (ii) the search is now correctly returning the same number of results when doing a list by property or a property search (duplicates are removed).

5. Research highlights (2013-2014)

The research highlights are discussed below in terms of new developments (results from completed PhD-projects) as well as publications record.

5.1 Summary of completed PhD research projects

5.1.1 Alberto Quagli*, 2013, "*An Integrated Business and Engineering Framework for Synthesis and Design of Processing Networks*", PhD-thesis (PEC13-41) – CAPEC*

The problem of synthesis and design of processing networks corresponds to the generation, evaluation and selection among alternatives with respect to raw materials, process technologies and configurations and product portfolio compositions. This results in a complex and multi-disciplinary problem, in which all the aspects of the problem (technical, economical, regulatory, logistical, etc.) need to be considered simultaneously, in order to be able to identify the optimal design.
Through the developments realized in the last decades, Process Systems Engineering has shown the potential to contribute to this problem, through the development of methods, tools, and solution approaches, under the general framework of Enterprise-Wide Optimization. Despite the level of maturity which these tools have reached and the potential which they have demonstrated, the acceptance of systematic methods and tools for synthesis and design of processing networks in the industrial sector is still lower than what could be expected. One of the key reasons for this lack of acceptance lays in their complexity. The formulation of these problems, in fact, often results in a time-consuming activity, due to the number of data that need to be gathered and of equations that need to be specified. The solution of the optimization problem formulated, moreover, requires expertise in discrete optimization, which is often not part of the standard skills set of design engineers and decision-makers.
This Ph.D. project, therefore, aims at the integration of methods, tools and solution strategies for synthesis and design of processing networks in a computer-aided framework, in order to optimize and facilitate the workflow of problem formulation and solution, allowing simpler, faster and more robust use of such tools. Through the integration of different methods, tools, algorithms and databases, the framework guides the user in dealing with the mathematical complexity of the problems, allowing efficient formulation and solution of large and complex optimization problem.

In this thesis, all developed methods, tools and solution strategies are described, emphasizing their integration in the computer aided framework. The framework is then applied to the formulation and solution of 3 challenging and relevant case studies, highlighting the importance of the tools integration realized in the framework.

5.1.2 Amol Shivajirao Hukkerikar, *2013,* "Development of pure component property models for chemical product-process design and analysis*", PhD-thesis (PEC13-42) - CAPEC*

Property prediction models based on the group-contribution+ (GC+) approach have been developed to provide reliable predictions of pure component properties together with uncertainties of predicted property values which is much needed information in performing chemical product and process design and analysis of sustainable chemical processes. For developing property models, a systematic methodology for property modeling and uncertainty analysis is employed. The methodology includes a parameter estimation step to determine parameters of the property model and an uncertainty analysis step to establish statistical information about the quality of parameter estimation, such as the parameter covariance, the standard errors in predicted properties, and the confidence intervals. For parameter estimation, large data sets of experimentally measured property values of a wide range of pure components taken from the CAPEC database, the US Environmental Protection Agency (EPA) database, and the USEtox database are used. In total, 21 thermo-physical properties and 22 environmental-related properties of pure components which include normal boiling point, critical constants, standard enthalpy of formation, liquid viscosity, fathead minnow 96-h LC50, oral rat LD50, global warming potential, emission to urban air (carcinogenic and noncarcinogenic) among others are modeled and analyzed. For all the estimated pure component properties, the corresponding 95% confidence intervals are also reported thereby providing information on the degree of accuracy of the property estimates. In addition, a method based on the 'molecular structural similarity criteria' is developed so that efficient use of knowledge of properties could be made in the development/improvement of property models. This method, in principle, can be applied to a wide range of properties of pure components. In this work, however, the application of 'molecular structural similarity criteria' is illustrated by considering performance improvement of models for enthalpy of formation, enthalpy of fusion, and critical temperature. For all properties listed above, it has been possible to achieve significant improvements in the performance of their models. The improved GC model for enthalpy of formation yields an average absolute deviation of 1.75 kJ/mol, which is well within the required *chemical accuracy*. Important issues related to property modeling such as: (i) quantity of property data used for the parameter regression; (ii) selection of the most appropriate form of the property model function; and (iii) the accuracy and thermodynamic consistency of predicted property values are also discussed. The developed models have been implemented into ProPred®, a property estimation toolbox of Integrated Computer Aided System, ICAS®, developed at CAPEC, DTU. Finally, a methodology for performing sensitivity analysis of process design due to uncertainties of property estimates is presented. This methodology allows the user to evaluate the effects of uncertainties of property estimates on the final design; list and rank properties that are most important from process design point of view; and establish acceptable levels of accuracy for property models. The application of this methodology is highlighted through three case studies namely, design of an extractive distillation process, design of a short-path evaporator, and design of a de-acidification system of vegetable oil deodorization process.

5.1.3 Anna Katrine Vangsgaard, 2013, "Modeling, Experimentation, and Control of Autotrophic Nitrogen Removal in Granular Sludge Systems", *PhD thesis (PEC13-50) - CAPEC*

Complete autotrophic nitrogen removal (CANR) is a novel process that can increase the treatment capacity for wastewaters containing high concentrations of nitrogen and low organic carbon to nitrogen ratios, through an increase of the volumetric removal rate by approximately five times. This process is convenient for treating anaerobic digester liquor, landfill leachate, or special industrial wastewaters, because costs related to the need for aeration and carbon addition are

lowered by 60% and 100%, respectively, compared to conventional nitrificationdenitrification treatment. Energy and capital costs can further be reduced by intensifying the process and performing it in a single reactor, where all processes take place simultaneously, e.g. in a granular sludge reactor, which was studied in this project. This process intensification means on the other hand an increased complexity from an operation and control perspective, due to the smaller number of actuators available.
In this work, an integrated modeling and experimental approach was used to improve the understanding of the process, and subsequently use this understanding to design novel control strategies, providing alternatives to the current ones available. First, simulation studies showed that the best removal efficiency was almost linearly dependent on the volumetric oxygen to nitrogen loading ratio. This finding among others, along with experimental results from start-up of lab-scale reactors, served as the basis for development of three single-loop control strategies, having oxygen supply as the actuator and removal efficiency as the controlled variable. These were investigated through simulations of an experimentally calibrated and validated model. A feedforward-feedback control strategy was found to be the most versatile towards the disturbances at the expense of slightly slower dynamic responses and additional complexity of the control structure. The functionality of this strategy was tested experimentally in a lab-scale reactor, where it showed the ability to reject disturbances in the incoming ammonium concentrations. However, during high ammonium loadings, when the capacity of the present sludge was reached, an oscillatory response was observed. Proper tuning of the controller is therefore of essential importance.
In this thesis, it was demonstrated that proactive use of model simulations, in an integrated methodology with experimentation, resulted in improved process understanding and novel control ideas. This will contribute to moving this promising technology from a case-by-case ad-hoc approach to a more systematic knowledge based approach.

5.1.4 Nor Alafiza Yunus, 2014, "Systematic Methodology for Design of Tailor-Made Blended Products: Fuels and Other Blended Products", *PhD Thesis (PEC14-19) - CAPEC*

A tailor-made blended liquid product is defined as a formulation of various chemicals in the liquid state to obtain a liquid mixture with a specific set of desired characteristics and qualities. Examples of blended liquid products are synthetic fuels and lubricants. This type of products is very important in daily life, since they not only keep people moving around, but also guarantee that machines and equipment work smoothly. The objective of this work is to tackle the blending problems using computer-aided tools for the initial stage of the product design.
A systematic methodology for design of tailor-made blended products has been developed, which has four main tasks. First, the design problem is defined: the product needs are identified, translated into target properties and the bounds for each target property are defined. Secondly, target property models are retrieved from a property model library. Thirdly, a mixture/blend design algorithm is applied to obtain the mixtures/blends that match the design targets. The result is a set of blends that match the constraints, the composition of the chemicals present in the blend, and the values of the target properties. Finally, the mixture target property values are verified by means of rigorous models for the properties and the mixtures. Besides the methodology, as the main contribution, specific supporting tools that were developed to perform each task are also important contributions of this research work.
The applicability of the developed methodology and tools was tested through two case studies. In the first case study, two different gasoline blend problems have been solved. In the second case study, four different lubricant design problems have been solved.

5.2 Publications Record

The last 12-months have seen a big increase for CAPEC in the number of peer-reviewed journal publications. 24+ published paper from 1 June 2013 to present (plus 29+ "in press" or "submitted") have been published in major chemical engineering journals (see Appendix 7.3). There have been 11 plenary or keynote lectures international conferences and 82+ presentations have been made in important international conferences during the period 1 January 2013 to 10 June 2014. This has given CAPEC greater visibility and attracted more attention to the research results published by CAPEC coworkers. CAPEC continues to have an open policy with respect to the publication of model parameters (especially, the CAPEC developed property models). The new version of ICAS 17.0 has all the latest property models and updated property model parameters.

6. Future Developments & Opportunities

For the industrial consortium, CAPEC and PROCESS are working on developing and analyzing new products and their corresponding processes together with achieving further process-product improvements through application of green chemistry principles and sustainability measures. Several joint-projects have been initiated to achieve this. First, however, a brief overview on PSE/CAPE and its relation to the CAPEC-PROCESS industrial consortium is given, followed by the current and future research plans within the identified focus areas.

6.1 Relation to PSE/CAPE

Process systems engineering promotes the solution of a problem in a systematic manner. In this way, although it has traditionally been applied by the chemical engineering community to solve problems for the oil and petrochemical industries, its potential application range is much wider. This is because the word "process" also implies, among others, the process of solving a problem; design of a biochemical/biological process for conversion of biomaterial to specific chemicals; and, the process of finding/designing chemicals with desired properties.

Most of the earlier developments can be linked to chemical processes involved with the manufacture of high volume bulk chemicals and the related industries (such as the oil and gas, petrochemical and chemical industries). To a lesser extent, these methods and tools have also been applied to the manufacture of low volume specialty chemicals. Since its formation, CAPEC has contributed by providing systematic, reliable and efficient models, methods and tools that have now become standard for the chemical process industries as well as in chemical engineering education. CAPEC software, employing CAPEC models and methods, such as ProPred (property prediction software), ProCAMD (molecular design-solvent selection software), SustainPro (sustainable process design software), ProCAFD (process flowsheet design/synthesis), ICAS (Integrated Computer Aided System), are routinely used by the CAPEC consortium members and close to 75 universities outside of Denmark.

The question therefore arises, what next? Where are the new challenges for CAPEC and what could be the new directions for research and education? Through collaboration with the CAPEC industrial member companies and academic partners, CAPEC conducted a "gap-analysis" with respect to identifying the current trends and the future needs with respect to chemical products, the processes that manufacture them and the models, methods and tools needed to design, analyze and operate them. The conclusions are briefly summarized below.

> *"To satisfy the needs of the modern society, it is necessary to continuously develop better and significantly improved chemicals based products. The bulk chemicals as well as the specialty chemicals have important roles. For example, the bulk chemicals act as raw materials, solvents, process fluids, etc., are needed in the manufacture of specialty*

chemicals that may become an active ingredient for a pharmaceutical and/or drug product. Therefore improved designs of continuous processes (needed for the manufacture of bulk chemicals) are as important as designs of batch operations (needed for the manufacture of specialty chemicals). Also, alternative production routes from renewable feed materials and retrofit of processes for changes in feed materials while focusing on energy, water and environmental issues will need special attention."

6.2 Future Plans

Based on the above, CAPEC-PROCESS research collaboration will address the following questions:

- How does one identify the chemicals and their synthesis routes that will help to meet future economic demands, taking into account, also the questions of sustainability and protection of the environment (*e.g.*, energy conservation and water resources)?
- How does one find their replacements for feedstocks and reagent as well as product and the processes to manufacture the products? The sources for many of the raw materials used, especially those derived from oil, gas, and some plants/animals continue to be depleted and may soon be economically infeasible to use (*e.g.*, bio-refinery and green chemistry).
- How to develop and provide the necessary models, methods and tools through which the future problems can be addressed (*e.g.*, multiscale modelling & integration/intensification)?

CAPEC and PROCESS plan to invest heavily in the following areas:

- Product-process modelling: Development of a generic computer aided modelling framework through which product-process models of different forms and scale can be generated/created while consuming significantly less time and resources than current practice.
- Product-process design: Use of a multi-disciplinary approach because the process-product knowledge (including data) will come from different sources and the performance criteria, factors, etc., will involve other research groups (expertise). The opportunity for CAPEC and PROCESS is that it can play the role of the "integrator" or "glue".
- Sustainable and greener process development: Develop systematic solution approaches that combine methods and tools from different sources into problem specific flexible, reliable and efficient systems.

More specifically, for CAPEC and PROCESS to meet the challenges for the future, the following topics will have higher priority:

- Computer aided frameworks for generation and use of multi-scale models (further extension of the predictive-generic property-product–process models)
- Methods for design of experiments to collect and analyze data (efficient use of resources in data collection) and, verification by experiments (through collaboration between CAPEC and PROCESS)
- Methods & tools for process-product monitoring/control systems (and their design)
- Sustainable process-product development (such as, hybrid processes, green chemistry, process intensification)
- Systematic methods for product discovery (further extension of computer aided molecular and mixture design)

- Evaluation of alternative processes for sustainability, retrofit and process modification
- Evaluation tools to identify biocatalytic process bottlenecks and strategies to improve the biocatalyst (in collaboration with others) and process

6.3 Managing the complexity through a systems approach

Product-process design and development in the life sciences, pharmaceutical, food and related industries, as opposed to the oil and petrochemical industries, is principally dependent on experiment-based trial and error approaches. Furthermore, unlike the oil and petrochemical industries in the life sciences, pharmaceutical, food and related industries, problems associated with product-process design and development involve, among others, the following distinct features:

- Multi-scale: important data related to the chemicals come from different sources, at different scales of time and size; for example, the properties that define the product characteristics are based on the microstructure of the molecule or material, while the process behaviour that needs to be monitored and controlled during operation is defined by the macroscopic (end-use) properties of the chemical system.
- Multidiscipline: the conversion of the biomaterial through biocatalysis requires knowledge of organic synthesis, enzymes, reaction catalysis, bioreactor design and operation – information about these topics come from different disciplines.
- Computer-aided techniques: lack of models to predict the behaviour of the chemicals at different scales, of enzymes during organic synthesis, of reaction kinetics, etc., means that appropriate model-based computer aided techniques have not been developed and use of experiment-based techniques is the only option.

Advances have been made on each of the above issues on specific areas of chemical and biochemical engineering. For example, multiscale polymerization reactors have been developed to investigate the operation of reactors; techno-economic assessment related to sustainability biofuels have been made using data from engineers, economists and scientists; computer-aided systems have been developed to perform routine mass and energy balances of chemical and biochemical processes. The demand for improved chemical-based products, made from more sustainable raw material resources and employing more efficient processes to make them, however, requires the above issues and others to be tackled in an integrated manner. This means that methods and tools suitable for current and future product-process development need to manage complex situations that require handling of data and knowledge from different sources and at different time and size scales. That is, the dimensions of the problems we need to solve have become larger. Therefore, a systems approach that can efficiently "manage the complexity" becomes very desirable.

In the multi-dimensional and multi-scalar nature of problems, at the micro- and meso- scales, the related problems are dealing with the microstructure of the molecules or materials and their properties; at the macro-scale (traditional area of application of chemical engineering), the related problems are mainly dealing with the process and its operation to produce a desired chemical; at the mega-scale, the related problems are, among others, dealing with enterprise wide optimization and supply chain issues. Many of the problems of current interest, such as, finding the optimal biorefinery, sustainable chemical process-product design, use of green solvents, process (energy and water) integration, etc., involve the macro- and mega-scales.

To manage the complexity, a systems approach would develop a framework (the architecture of the software) for handling the diverse set of methods and tools needed to solve a wide range of problems, for a potential computer-aided system. Such systems need to have a knowledge base of data (for example, of the active ingredients, solvents, polymers, etc.); a library of models (for example, models to predict properties – in case data is not available - of active ingredients, solvents, polymers, etc.; models to predict the controlled release from the microcapsule; models to predict the

behaviour of the mixing process); a design method (for example, guiding the engineer/scientist through the sequence of steps needed to identify the best solution); and, other associated methods-tools (such as a tool to analyze data; a tool to create the missing model; a tool to screen feasible alternatives). The principal idea here is to decompose a complex problem into a set of sub-problems that are easier to solve and identify those that can be solved through model-based solution approaches. Solving these sub-problems according to a pre-determined sequence helps to reduce the search space through each subsequent sub-problem solution, until a sub-problem cannot be solved with models anymore. At this point, the experiment-based trial and error approach takes over to determine the final solution. The advantage of this combined hybrid (systems approach) is that during the early stages, where enough data and models are available (or could be easily generated), the search space is rapidly reduced. In the later stages, where quantitative values become important and data/models become more unreliable, the experimental resources are employed, sometimes only to evaluate a few feasible alternatives to identify the truly innovative and best solution. Several examples of such computer aided systems can be found at CAPEC and current research is expanding on this approach through the development of a collection of methods and tools.
An example of managing the complexity is shown through Fig 5.1, where a common decomposed framework is highlighted for computer adied molecular design (CAMD) and computer aided flowsheet design (CAFD).

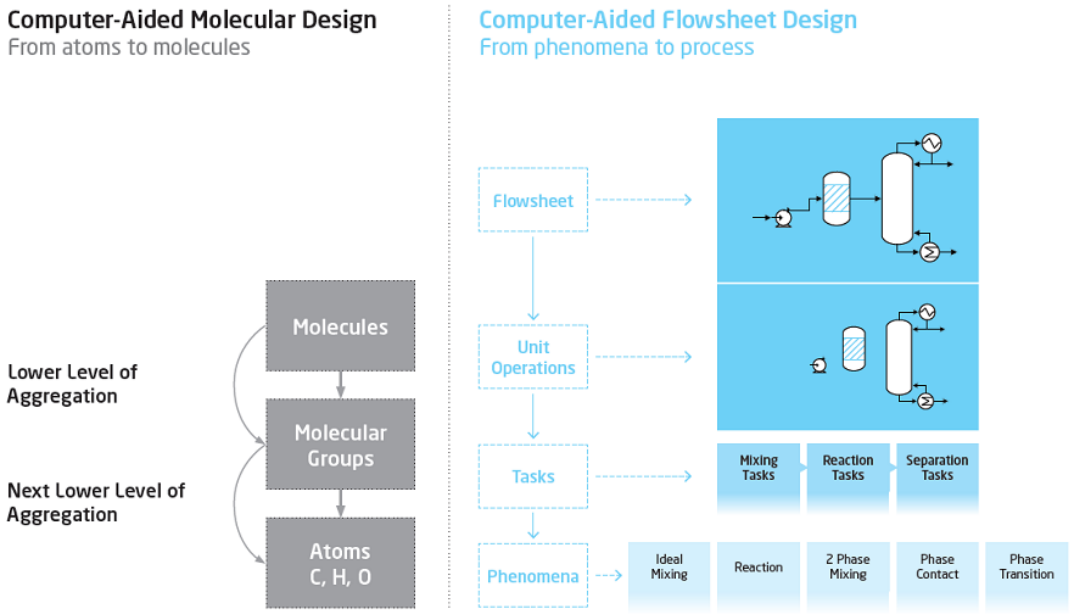


Figure 5.1: Multiscale nature of product-process design problems

6.4 Some specific plans (CAPEC-PROCESS coworkers) for the future

Major collaboration between CAPEC and PROCESS will be established in the areas of thermodynamics of biocatalytic processes; in the development of generic process plants and in the development of the integrated biorefinery concept. At the same time, the current collaboration between CAPEC and PROCESS in the areas of crystallization modeling, control and monitoring; tailor-made blend design; process intensification; control and monitoring of biodiesel processes, and wastewater management will be continued. Collaboration with member companies in the areas of property prediction; process synthesis, design and intensification; solvents; integrated economic-business solutions; and the development of model based applications will continue. Specific projects in the areas of computer aided molecular and blend design; integrated biorefinery; water networks; process intensification and properties prediction are also set-up with collaboration partners from academia.

7. Appendix

7.1 PROCESS lab and Pilot plant

The PROCESS experimental facilities are based in two laboratories in building 227 – one for biocatalysis and one for fermentation – and also the pilot hall in building 228. The possibility of batch, fed-batch and continuous process operations of biocatalytic reactions at miniature, lab and pilot scale is being developed. Both packed bed and stirred reactors are available. Batch and fed-batch fermentations can be operated at lab scale and pilot scale, while a new reactor design for small-scale fermentations (V = 1 ml) is under development.. Analytical equipment is in place.

Figure 7.1: The main laboratory of the Process group

Figure 7. 2: One of the HPLC setups

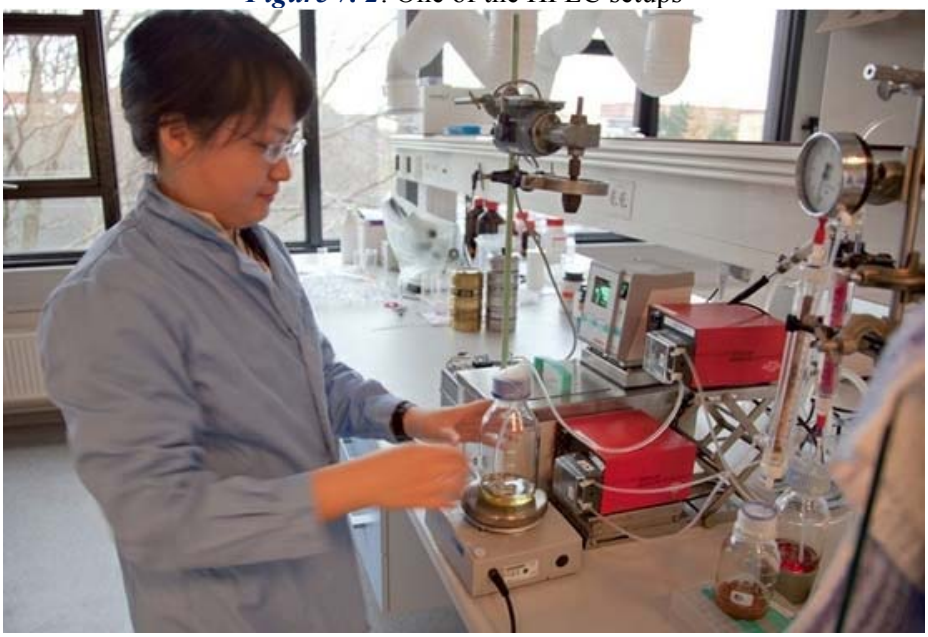


Figure 7.3: The former PhD student Yuan Xu is producing Biodiesel in a Batch Reactor

Figure 7.4: A group of students discussing the enjoyable latest results

7.2 CAPEC Control Lab

The main purpose of the CAPEC Control Lab is to give our students hands-on experience with process control problems. The laboratory is presently undergoing a complete renovation.

Two facilities are in use:

- a 4-tank exercise, and
- a distillation column

With the 4-tank exercise (used as a 2-tank system), students make two experiments. The first day they determine the dynamics of the system. Then they go to the computer lab to configure a PI-controller by simulation. On the second day they try out their controller settings on the real system. This setup is used in all our introductory teaching; about 75 students each year.

A HTST pasteurizer has also been established

The distillation column is used in an intensive 3-weeks course where the participants are taught to:
- Plan and execute start-up of the chemical plant.
- Apply a Distributed Control System for chemical plant operation.
- Simulate and document the operation of a chemical plant.
- Reason on process behaviour during start-up and operation.


4 tank exercise


HTST pasteurizer


Indirect Vapour Recompression Distillation Pilot Plant

7.3 Publication list (1 June 2013 – 10 June 2014)

Publications listed under PECxx-yy indicate CAPEC publications where one or more authors are CAPEC members, whether or not PROCESS is involved. Publications listed under PROCESS indicate PROCESS publications where there is no joint activity with CAPEC.

	A - Ph.D. Theses and Monographs
PEC13-41	Alberto Quaglia, 2013, "An Integrated Business and Engineering Framework for Synthesis and Design of Processing Networks", Ph.D thesis
PEC13-42	Amol Shivajirao Hukkerikar, 2013, "Development of pure component property models for chemical product-process design and analysis", Ph.D. thesis
PEC13-50	Anna Katrine Vangsgaard, 2013, "Modeling, Experimentation, and Control of Autotrophic Nitrogen Removal in Granular Sludge Systems", Ph.D. thesis
PEC13-63	Abildskov J., Wedberg R., O'Connell J.P., 2013, "Fluctuation Solution Theory Properties from Molecular Simulation" in "Fluctuation Theory of Solutions: Applications in Chemistry, Chemical Engineering and Biophysics", Ch. 6. Edited by Matteoli E., O'Connell J.P., Smith P.E., CRC Press, Taylor & Francis Group. ISBN: 978-1-43-989922-9 (Hardback)
PEC13-64	Abildskov J., O'Connell J.P., 2013, "Molecular Thermodynamic Modeling of Fluctuation Solution Theory Properties" in "Fluctuation Theory of Solutions: Applications in Chemistry, Chemical Engineering and Biophysics", Ch. 9. Edited by Matteoli E., O'Connell J.P., Smith P.E., CRC Press, Taylor & Francis Group. ISBN: 978-1-43-989922-9 (Hardback)
PEC14-10	Klaus Reinholdt Nyhuus Hansen, **2014**, "New product introduction in the pharmaceutical industry", Ph.D. Thesis
PEC13-41	Alberto Quaglia, 2013, "An Integrated Business and Engineering Framework for Synthesis and Design of Processing Networks", Ph.D thesis
PEC13-42	Amol Shivajirao Hukkerikar, 2013, "Development of pure component property models for chemical product-process design and analysis", Ph.D. thesis
PEC14-19	Nor Alafiza Yunus, **2014**, "Systematic Methodology for Design of Tailor-Made Blended Products: Fuels and Other Blended Products", Ph.D. Thesis

	B - Reviewed publications in International Journals
PEC13-15	Vangsgaard, A.K., Mutlu, A.G., Gernaey, K.V., Smets, B.F. & Sin, G., 2013, "Calibration and validation of a model describing complete autotrophic nitrogen removal in a granular SBR system", Journal of Chemical Technology & Biotechnology, 88(11), 2007-2015
PEC13-17	P. Cheali, A. Quaglia, K. V. Gernaey, G. Sin, **2014**, "Effect of market price uncertainties on the design of optimal biorefinery systems - a systematic approach", Ind. Eng. Chem. Res., 53, pp. 6021−6032
PEC13-18	Amol S. Hukkerikar; Robert J. Meier, Gürkan Sin, Rafiqul Gani, 2013, "A Method to Estimate the Enthalpy of Formation of Organic Compounds with Chemical Accuracy", Fluid Phase Equilibria, 348, pp. 23-32
PEC13-20	Vangsgaard, A.K., Mauricio-Iglesias, M., Valverde-Perez, B., Gernaey, K.V. & Sin, G., 2013, "pH variation and influence in an autotrophic nitrogen removing biofilm system using an efficient numerical solution strategy", Water Science and Technology, 67(11), 2608-2615
PEC13-26	Singh R., Godfrey A., Gregertsen B., Muller F., Gernaey K.V., Gani R. and Woodley J.M., 2013, "Systematic substrate adoption methodology (SAM) for future flexible, generic pharmaceutical production processes", Computers and Chemical Engineering, 58, pp. 344-368

PEC13-36	Seyed Soheil Mansouri, Muhammad Imran Ismail, Deenesh K. Babi, Lida Simasatitkul, Jakob K. Huusom and Rafiqul Gani, 2013, "Systematic Sustainable Process Design and Analysis of Biodiesel Processes", Processes, 1, pp. 167-202
PEC13-37	Alberto Quaglia, Alessandra Pennati, Milos Bogataj, Zdravko Kravanja, Gürkan Sin, Rafiqul Gani, **2014**, "Industrial process water treatment and reuse: A framework for synthesis and design", Industrial & Engineering Chemistry Research, Vol. 53, p. 5160−5171
PEC13-38	Michele Mattei, Georgios M. Kontogeorgis and Rafiqul Gani , 2013, "Modeling of the Critical Micelle Concentration (CMC) of Nonionic Surfactants with an Extended Group-Contribution Method", Ind. Eng. Chem. Res., 52 (34), pp. 12236–12246
PEC13-47	Michele Mattei, Georgios M. Kontogeorgis, Rafiqul Gani, **2014**, "A Comprehensive Framework for Surfactant Selection and Design for Emulsion Based Chemical Product Design", Fluid Phase Equilibria, 362, pp. 288-299
PEC13-48	Larissa P.Cunico, Roberta Ceriani, Bent Sarup, John P. O'Connell, Rafiqul Gani, **2014**, "Data, analysis, modeling, and prediction of properties and phase equilibria for process design of edible oil and biodiesel systems", Fluid Phase Equilibria, 363, pp. 318-327
PEC13-49	A. G. Mutlu, A. K. Vangsgaard, G. Sin and B. F. Smets, 2013, "An operational protocol for facilitating start-up of single-stage autotrophic nitrogen-removing reactors based on process stoichiometry", Water Science and Technology 68(3), pp. 514-521
PEC13-53	John Villadsen, Sten Bay Jørgensen, **2014**, "Reflections on the aerobic fermentation stoichiometry of Crabtree positive yeasts", Biotechnology and Bioengineering, 111(3), pp. 632-637
PEC13-54	Peam Cheali, Krist V. Gernaey and Gürkan Sin, **2014**, "Toward a Computer-Aided Synthesis and Design of Biorefinery Networks: Data Collection and Management Using a Generic Modeling Approach", ACS Sustainable Chem. Eng., 2, pp. 19−29
PEC13-55	Remus Mihail Prunescu, Gürkan Sin, 2013, "Dynamic modeling and validation of a lignocellulosic enzymatic hydrolysis process – A demonstration scale study", Bioresource Technology 150C, pp. 393-403
PEC13-56	Muhammad Rizwan, Jay H. Lee, Rafiqul Gani. 2013, "Optimal processing pathway for the production of biodiesel from microalgal biomass: A superstructure based approach", Computers and Chemical Engineering, 58, pp. 305-314
PEC13-60	Dennis Bonné, María Antonieta Alvarez and Sten Bay Jørgensen, 2013, "Data Driven Modeling for Monitoring and Control of Industrial Fed-batch Cultivations", Industrial Engineering Chemistry Research, http://dx.doi.org/10.1021/ie402532t
PEC13-61	Herslund P.J., Thomsen K., Abildskov J., von Solms N., Galfréc A., Brântuas P., Kwaterski M., Herri J.-M., 2013, "Thermodynamic promotion of carbon dioxide–clathrate hydrateformation by tetrahydrofuran, cyclopentane and their mixtures", International Journal of Greenhouse Gas Control, 17, pp. 397-410
PEC13-62	Herslund P.J., Thomsen K., Abildskov J., Von Solms N., 2013, "Application of the cubic-plus-association (CPA) equation of state to model the fluid phase behaviour of binary mixtures of water and tetrahydrofuran", Fluid Phase Equilibria, 356, pp. 209-222
PEC13-65	Elham Ramin, Xavier Flores-Alsina, Gürkan Sin, Krist V. Gernaey, Ulf Jeppsson, Peter Steen Mikkelsen, Benedek Gy. Plósz, **2014**, "Influence of selecting secondary settling tank sub-models on the calibration of WWTP models - a global sensitivity analysis using BSM2", Chemical Engineering Journal, Vol. 241, pp. 28-34
PEC13-67	Nor Alafiza Binti Yunus; Krist V Gernaey; John M Woodley; Rafiqul Gani, **2014**, "A systematic methodology for design of tailor-made blended products", ESCAPE-23 Special Issue, Computers & Chemical Engineering, Vol 66, pp. 201-213

PEC14-01	Sawitree Kalakul, Pomthong Malakul, Kitipat Siemanond, Rafiqul Gani, **2014**, "Integrated of Life Cycle Assessment Software with Tools for Economic and Sustainability Analysis and Process Simulation for Sustainable Process Design", Journal of Cleaner Production, Vol 71, pp. 98-109
PEC14-02	Azizul Azri Bin Mustaffa, Rafiqul Gani, Georgios M. Kontogeorgis, **2014**, "Development and analysis of the original UNIFAC-CI model for prediction of vapor-liquid and solid-liquid equilibria", Fluid Phase Equilibria, 366, pp. 24-44
PEC14-16	Quaglia, A.; Gargalo, C.L.; Chairakwangsa, S.; Sin, G.; Gani, R.; **2014**, "Systematic network synthesis and design: problem formulation, superstructure generation, data management and solution", Computers & Chemical Engineering, Special Issue: Ignacio Grossmann, In Press, **DOI:** 10.1016/j.compchemeng.2014.03.007
PEC14-20	Anna Katrine Vangsgaard, Miguel Mauricio-Iglesias, Krist V. Gernaey, Gürkan Sin, **2014**, "Development of novel control strategies for single-stage autotrophic nitrogen removal: A process oriented approach", Computers & Chemical Engineering, DOI: http://dx.doi.org.globalproxy.cvt.dk/10.1016/j.compchemeng.2014.01.017

	B - Reviewed publications in International Journals - PROCESS
PRO14-01	Flores-Alsina X., Arnell M., Amerlinck Y., Corominas Ll., Gernaey K.V., Guo L., Lindblom E., Nopens I., Porro J., Shaw A., Snip L., Vanrolleghem P.A. and Jeppsson U., 2014, "Balancing effluent quality, economical cost and greenhouse gas emissions during the evaluation of (plant-wide) wastewater treatment control/operational strategies", Science of the Total Environment, 466-467, pp. 616-624
PRO14-02	Ramin E., Flores-Alsina X., Sin G., Gernaey K.V., Jeppsson U., Mikkelsen P.S. and Plósz B.G., 2014, "Influence of selecting secondary settling tank sub-models on the calibration of WWTP models – A global sensitivity analysis using BSM2", Chemical Engineering Journal, 241, pp. 28-34
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PRO14-06	Mortier S.T.F.C., Gernaey K.V., De Beer T. and Nopens I., 2014, "Analysing drying unit performance in a continuous pharmaceutical manufacturing line by means of mass – energy balances", European Journal of Pharmaceutics and Biopharmaceutics, 86, pp. 532-543
PRO14-07	Mortier S.T. F.C., Gernaey K.V., De Beer T. and Nopens I., 2014, "Global Sensitivity Analysis Applied to Drying Models for One or a Population of Granules", AIChE Journal, 60, pp. 1700-1717
PRO14-08	Olsson G., Carlsson B., Comas J., Copp J., Gernaey K.V., Ingildsen P., Jeppsson U., Kim C., Rieger L., Rodríguez-Roda I., Steyer J.-P., Takács I., Vanrolleghem P.A., Vargas A., Yuan Z., Åmand L., 2014, "Instrumentation, Control and Automation in wastewater – from London 1973 to Narbonne 2013", Water Science and Technology, 69, pp. 1373-1385

PRO14-09	Tufvesson, Pär; Bach, Christian; Woodley, John, 2014, **"**A model to assess the feasibility of shifting reaction equilibrium by acetone removal in the transamination of ketones using 2-propylamine**",** Biotechnology and Bioengineering, 111(2), pp. 309-319
PEC14-10	Hemalata Ramesh, John M. Woodley, 2014, " Process characterization of a monoamine oxidase", Journal of Molecular Catalysis B: Enzymatic, Accepted, http://dx.doi.org/ 10.1016/j.molcatb.2014.04.009

	C - In press/Submitted Manuscripts
PEC13-23	Singh, R., Godfrey, A., Gregertsen, B., Muller, F., Vankayala, B., Haas-Santo, K., Gernaey, K. V., Gani, R., Woodley, J. M., 2013, "Design of a process template for amine synthesis", Organic Process Research & Development, Submitted
PEC13-24	Singh, R., Gregertsen, B., Muller, F., Gernaey, K. V., Gani, R., Woodley, J. M., 2013, "Use of operating windows for assessment of continuous plug flow slurry reactor", AIChE Journal, Submitted
PEC13-40	Jason Price, Mathias Nordblad, John M. Woodley, Jakob K. Huusom, 2013, "Uncertainty and Sensitivity Analysis Applied to a Kinetic Model for Enzymatic Biodiesel Production", Bioprocess and Biosystems Engineering, Submitted
PEC13-46 Book cph.	Alicia Roman-Martinez, John M Woodley, Rafiqul Gani, 2013, "Design of novel integrated pharmaceutical processes: A model-based approach", In "Advances in Quality by Design", Editors: GV Reklaitis, C Seymore, Wiley, USA, In Press
PEC13-57	Jakob Kjøbsted Huusom og John Bagterp Jørgensen., **2014**, "A Realistic Process Example for MIMO MPC based on Autoregressive Models", Proceedings of 19th World Congress of the International Federation of Automatic Control (IFAC'14), Accepted
PEC13-58	Jason Price, Mathias Nordblad, John M. Woodley, Jakob K. Huusom, **2014**, "Fed-Batch Feeding Strategies for Enzymatic Biodiesel Production", Proceedings of 19th World Congress of the International Federation of Automatic Control (IFAC'14), Accepted
PEC13-59	Harald Waschl, John Bagterp Jørgensen, Jakob Kjøbsted Huusom, Luigi del Re, **2014**, "Conditional Reference Adaptation for Offset-free MPC", Proceedings of 19th World Congress of the International Federation of Automatic Control (IFAC'14), Accepted
PEC13-66	Chien-Tai Tsai, Ricardo Morales-Rodriguez, Gürkan Sin, Anne S. Meyer, 2013, "A Dynamic Model for Cellulosic Biomass Hydrolysis: A Comprehensive Analysis and Validation of Hydrolysis and Product Inhibition Mechanisms", Applied Biochemistry and Biotechnology, Accepted
PEC14-05	Hande Bozkurt, Alberto Quaglia, Krist V. Gernaey and Gürkan Sin, **2014**, "Superstructure Development and Optimization under Uncertainty for Design & Retrofit of Municipal Wastewater Treatment Plants", Proceedings for ESCAPE 24, Submitted
PEC14-09	Peam Cheali, Alberto Quaglia, Krist V. Gernaey, Gürkan Sin, **2014**, "Uncertainty analysis in raw material and utility cost of biorefinery synthesis and design", Proceedings for ESCAPE 24, Accepted
PEC14-11	Pichayapan Kongpanna, Varong Pavarajarn, Rafiqul Gani, Suttichai Assabumrungrat, **2014**, "Techno-economic evaluation of different CO2-based processes for dimethyl carbonate production", Chemical Engineering Research & Design, Submitted
PEC14-12	Marina Fedorova, Emmanouil Papadakis, Kresten T. Meisler, Gürkan Sin, Rafiqul Gani, **2014**, "Application of the Generic Modeling Template Approach to Unsaturated Fatty Acid Oxidation and Crystallization Systems", Proceedings for FOCAPD, Submitted

PEC14-13	Amata Anantpinijwatna, Gürkan Sin, John P. O'Connell, Rafiqul Gani, **2014**, "A Framework for the Modelling of Biphasic Reacting Systems", Proceedings for FOCAPD, Submitted
PEC14-14	Daniela de Faria, Alberto Quaglia, Fernando Pessoa, Rafiqul Gani, **2014**, "Early Stage Design of a Biorefinery from Castor Oil", Proceedings for FOCAPD, Submitted
PEC14-15	Deenesh K. Babi, Johannes Holtbruegge, Philip Lutze, Andrzej Górak, John M. Woodley, Rafiqul Gani, **2014**, "Sustainable Process Synthesis-Intensification", Proceedings for FOCAPD, Submitted
PEC14-17 Book Chapter	Deenesh K. Babi and Rafiqul Gani, **2014**, "Hybrid Distillation Schemes: Design, Analysis & Application", Chapter 9, in "Distillation, Fundamentals and Principles", Editors: A. Górak and E. Sorensen, Publisher: Elsevier, Submitted
PEC14-18	Kresten Meisler, Nicolas von Solms, Krist V. Gernaey, Rafiqul Gani, 2014, "Crystallization Kinetics within a Generic Modelling Framework", Chemical Engineering & Technology, Submitted
PEC14-21 Book Chapter	Peam Cheali, Alberto Quaglia, Carina L. Gargalo, Krist V. Gernaey, Gürkan Sin and Rafiqul Gani, 2014, "Early stage design and analysis of biorefinery networks", Book Chapter, *Process Design Strategies for Biomass Conversion Systems* (John Wiley & Sons, Inc.), Submitted
PEC14-22	Babi, D. K., Lutze, P., Woodley, J. M., Gani, R., 2014, "A Process Synthesis-Intensification Framework for the Development of Sustainable Membrane-based Operations", Chemical Engineering and Processing: Process Intensification, Submitted
PEC14-23	Mauricio-Iglesias, M. Huusom, J.K., Gernaey, K.V., 2014, "Intuitive examples of frequency response analysis for chemical engineers", Education for Chemical Engineers, Submitted
PEC14-24	Miguel Mauricio-Iglesias; Ignacio Montero-Castro; Ane L Mollerup; Gürkan Sin, 2014, "Self-optimising control of sewer systems. A generic methodology", Environmental Management, Submitted
PEC14-26	Miguel Mauricio-Iglesias, Anna-Katrine Vangsgaard, Krist V Gernaey, Barth F Smets, Gürkan Sin, 2014, "A novel control strategy for single-stage autotrophic nitrogen removal in SBR", Chemical Engineering Journal, Submitted
PEC14-27	Miguel Mauricio-Iglesias, Thomas Bisgaard, Henrik Kristensen, Krist V. Gernaey, Jens Abildskov, Jakob K. Huusom, 2014, "Pressure control in distillation columns. A model-based analysis", IECR, Submitted
PEC14-29	Jason Price, Björn Hofmann, Vanessa T. L. Silva, Mathias Nordblad, John M. Woodley, Jakob K. Huusom, 2014, "Mechanistic Modelling of Biodiesel Production using a Liquid Lipase Formulation", Biotechnology Progress, Submitted
PEC14-30	R. Boiocchi, M. Mauricio-Iglesias, A.K. Vangsgaard, K.V. Gernaey, G. Sin, 2014, "A fuzzy-logic based diagnosis and control of a reactor performing complete autotrophic nitrogen removal", Journal of Process Control, Submitted
PEC14-31	Rafiqul Gani, Ka M. Ng, 2014, "Product Design - From Molecules to Formulations to Devices", Proceedings for FOCAPD, Submitted
PEC14-32	Peter Lützen, Miguel Mauricio-Iglesias, Jakob Kjøbsted Huusom, Jens Abildskov, 2014, "Control Benchmark for Solvent Recovery by Distillation", Proceedings for 10th International Conference on Distillation & Absorption 2014
PEC14-33	Abildskov J., O'Connell J.P., 2014, " On the Responses of Azeotropes to Pressure Variations ", Proceedings for 10th International Conference on Distillation & Absorption 2014

PEC14-34	Meyer K., Ianniciello L., Nielsen J.E., Bisgaard T., Huusom J.K., Abildskov J., 2014, "HIDiC - Design, Sensitivity and Graphical Representation", Proceeding for 10th International Conference on Distillation & Absorption 2014
PEC14-35	Thomas Bisgaard, Jakob Kjøbsted Huusom, Jens Abildskov, 2014, "Impact on Model Uncertainty of Diabatization in Distillation Columns", Proceedings for 10th International Conference on Distillation & Absorption 2014
PEC14-36 Book Chapter	Rafiqul Gani, Deenesh K Babi, 2014, "Systematic computer aided framework for process synthesis, design and intensification", in "Chemical Processes for a Sustainable Future", Trevor Letcher - Editor, Royal Society of Chemistry, UK, In Press

	D - Reviewed Conference Proceedings
PEC12-43	Daniel Haugaard Olesen, Jakob Kjøbsted Huusom, John Bagterp Jørgensen, 2013, "Tuning Procedure for ARX-based MPC of Multivariate Processes", Proceedings of American Control Conference (ACC), pp. 1724-1729
PEC13-04	Peam Cheali, Krist V. Gernaey and Gürkan Sin, 2013, "Synthesis and design of optimal biorefinery using an expanded network with thermochemical and biochemical biomass conversion platforms", Computer-Aided Chemical Engineering Series, Volume 32, pp. 985-990
PEC13-05	Nor Alafiza Yunus, Krist V. Gernaey, John M. Woodley and Rafiqul Gani, 2013, "Design of Sustainable Blended Products using an Integrated Methodology", Computer-Aided Chemical Engineering Series, Volume 32, pp. 835-840
PEC13-06	Marina Fedorova, Gurkan Sin, Rafiqul Gani, 2013, "Computer-aided modeling framework – a generic modeling template for catalytic membrane fixed bed reactors", Computer-Aided Chemical Engineering Series, Volume 32, pp. 775-780
PEC13-07	Anna Katrine Vangsgaard, Miguel Mauricio-Iglesias, Krist V. Gernaey, Barth F. Smets, Gürkan Sin, 2013, "Control of a Biological Nitrogen Removal Process in an Intensified Single Reactor Configuration", Computer-Aided Chemical Engineering Series, Volume 32, pp. 769-774
PEC13-08	Alberto Quaglia, Bent Sarup, Gürkan Sin, Rafiqul Gani, 2013, "Design of a Generic and Flexible Data Structure for Efficient Formulation of Large Scale Network Problems", Computer-Aided Chemical Engineering Series, Volume 32, pp. 661-666
PEC13-09	Michele Mattei, Michael Hill, Georgios M. Kontogeorgis, Rafiqul Gani, 2013, "Design of an Emulsion-based Personal Detergent through a Model-based Chemical Product Design Methodology", Computer-Aided Chemical Engineering Series, Volume 32, pp. 817-822
PEC13-10	Thomas Bisgaard, Jakob Kjøbsted Huusom, Jens Abildskov, 2013, "Dynamic effects of diabatization in distillation columns", Computer-Aided Chemical Engineering Series, Volume 32, pp. 1015-1020
PEC13-19	Remus Mihail Prunescu, Jakob Munch Jensen, Mogens Blanke and Gürkan Sin, 2013, "Modelling and L1 Adaptive Control of pH in Bioethanol Enzymatic Process", Proceedings of 2013 American Control Conference (ACC), pp. 1888-1891
PEC13-21	Jing Wu, Laibin Zhang, Morten Lind, Wei Liang, Jinqiu Hu, Sten Bay Jørgensen, Gürkan Sin, Zia Ullah Khokhar, 2013, "Hazard Identification of the Offshore Three-phase Separation Process Based on Multilevel Flow Modeling and HAZOP", Proceedings of The 26th International Conference on Industrial, Engineering & Other Applications of Applied Intelligent Systems (IEA/AIE), Lecture Notes in Computer Science Volume 7906, pp 421-430
PEC13-22	Daniel Haugaard Olsen, Jakob Kjøbsted Huusom, John Bagterp Jørgensen, 2013, "A Tuning Procedure for ARX-based MPC", Proceedings of the IEEE Multi-conference on Systems and Control (MSC2013), pp. 188-193

PEC13-27	S. Mangnimit, P. Malakul , R. Gani, 2013, "Sustainable Process Design of Biofuels: Bioethanol Production from Cassava rhizome", Proceedings of the 6th International Conference on Process Systems Engineering (PSE ASIA), pp. 910-913
PEC13-29	Sawitree Kalakul, Pomthong Malakul', Kitipat Siemanond, and Rafiqul Gani, 2013, "Software Integration of Life Cycle Assessment and Economic Analysis for Process Evaluation", Proceedings of the 6th International Conference on Process Systems Engineering (PSE ASIA), pp. 917-922
PEC13-31	Mauricio-Iglesias, M.; Vangsgaard, A.K.; Gernaey, K.V.; Sin, G., 2013, "A fuzzy-logic based diagnosis and control of a reactor performing complete autotrophic nitrogen removal", Proceedings of 12th IFAC Symposium on Computer Applications in Biotechnology (CAB 2013), pp. 205-210
PEC13-32	Mauricio-Iglesias, M.; Montero-Castro, I.; Mollerup, A.L.; Sin, G., 2013, "Self-optimising control of sewer systems", Proceedings of 10th International IFAC Symposium on Dynamics and Control of Process Systems (DYCOPS 2013), pp. 708-712
PEC13-33	Jason Price, Mathias Nordblad, John M. Woodley, Jakob K. Huusom, 2013, "Application of Uncertainty and Sensitivity Analysis to a Kinetic Model for Enzymatic Biodiesel Production", Proceedings of 12th IFAC Symposium on Computer Applications in Biotechnology (CAB 2013), 12(1), pp. 161-168
PEC13-34	Thomas Bisgaard, Jakob Kjøbsted Huusom and Jens Abildskov, 2013, "A Modeling Framework for Conventional and Heat Integrated Distillation Columns", Proceedings of 10th International IFAC Symposium on Dynamics and Control of Process Systems (DYCOPS 2013), pp. 373-378
PEC13-43	Noor Asma Fazli Abdul Samad, Gürkan Sin, Krist V. Gernaey, Rafiqul Gani, 2013, "Designing Robust Process Analytical Technology (PAT) Systems for Crystallization Processes: A Potassium Dichromate Crystallization Case Study", Proceedings of the 6th International Conference on Process Systems Engineering (PSE ASIA), pp. 207-212
PEC13-44	Noor Asma Fazli Abdul Samad, Gürkan Sin, Krist V. Gernaey, Rafiqul Gani, 2013, "A Robust Process Analytical Technology (PAT) System Design for Crystallization Processes", Proceedings of 20th International Workshop on Industrial Crystallization (BIWIC2013), pp. 1-8
PEC13-45	Niels Jensen, Sten Bay Jørgensen, 2013, "Learning Safety Assessment from Accidents in a University Environment", Chemical Engineering Transactions 31, The Italian Association of Chemical Engineering, pp. 427-432
PEC13-51	Kresten T. Meisler, Nicolas von Solms, Krist V. Gernaey, Rafiqul Gani, 2013, "Crystallization Kinetics within a Generic Modelling Framework", Proceedings of 20th International Workshop on Industrial Crystallization (BIWIC2013), pp. 176-183
PEC13-52	Remus Mihail Prunescu, Mogens Blanke and Gürkan Sin, 2013, "Modelling and L1 Adaptive Control of Temperature in Biomass Pretreatment", Proceedings of 52nd IEEE Conference on Decision and Control, pp. 1-8
PEC13-68	Muhammad Rizwan, Jay H. Lee, Rafiqul Gani, 2013, "Superstructure optimization of biodiesel production from microalgal biomass", Proceedings of 10th International IFAC Symposium on Dynamics and Control of Process Systems (DYCOPS 2013), pp. 111-116
D PEC14-03	Alberto Quaglia, Gürkan Sin, Rafiqul Gani, **2014**, "Financial risk analysis in the synthesis and design of processing networks: Balancing risk and return", Computer Aided Chemical Engineering, Vol. 33, pp. 1-6
D PEC14-04	Michele Mattei, Nor A. Yunus, Sawitree Kalakul, Georgios M. Kontogeorgis, John M. Woodley, Krist V. Gernaey, Rafiqul Gani, **2014**, "The Virtual Product-Process Design Laboratory for Structured Chemical Product Design and Analysis", Computer Aided Chemical Engineering, Vol. 33, pp. 61-66

PEC14-06	Carina L. Gargalo, Ana Carvalho, Henrique A. Matos, Rafiqul Gani, **2014**, "Techno-Economic, Sustainability & Environmental Impact Diagnosis (TESED) Framework", Computer Aided Chemical Engineering, Vol. 33, pp. 1021-1026
PEC14-07	Marina Fedorova, Gürkan Sin, Rafiqul Gani, **2014**, "Computer-Aided Template for Model Reuse, Development and Maintenance", Computer Aided Chemical Engineering, Vol. 33, pp. 817-822
PEC14-08	D. K. Babi, J. M. Woodley, R. Gani, **2014**, "Achieving More Sustainable Designs through a Process Synthesis-Intensification Framework", Computer Aided Chemical Engineering, Vol. 33, pp. 31-36
PEC14-28	Bozkurt H., Quaglia A., Gernaey K.V. and Sin G., **2014**, "Early-stage design of municipal wastewater treatment plants – presentation and discussion of an optimisation based concept", in Proc. 4th IWA/WEF Wastewater Treatment Modelling Seminar (WWTmod2014), pp. 254-257

	E - Other Publications & Reports
PEC13-13	Ane Loft Mollerup, Morten Grum, Dirk Muschalla, Edwin van Velzen, Peter Vanrolleghem, Peter Steen Mikkelsen and Gurkan Sin, 2013, "Integrated control of the wastewater system – potentials and barriers", Water21, April 2013 (15.2), pp 39-41
PEC13-25	Rafiqul Gani and John Woodley, 2013, "CAPEC-PROCESS Research Report 2013", CAPEC-PROCESS Internal Report, DTU-KT, Lyngby, Denmark
PEC13-28	Saranya Mangnimit, Pomthong Malakul, and Rafiqul Gani, 2013, "Sustainable Process Design of Lignocellulose based Biofuel", Proceedings of WCCE9 & APCChE 2013
PEC13-30	Sawitree Kalakul, Pomthong Malakul, Kitipat Siemanond, Rafiqul Gani, 2013, "A Generic Life Cycle Assessment Tool For Chemical-biochemical Processes", Proceedings of WCCE9 & APCChE 2013
PEC13-39	Amol S. Hukkerikar, Bent Sarup, Gürkan Sin, and Rafiqul Gani, 2013, "Molecular structure based property modeling: Development/ improvement of property models through a systematic property-data-model analysis", Proceedings of PPEPPD-2013, Submitted
PEC14-25	Rafiqul Gani and John Woodley, 2014, "CAPEC-PROCESS Research Report 2014", CAPEC-PROCESS Internal Report, DTU-KT, Lyngby, Denmark
	Thomas Bisgaard, Jakob Kjøbsted Huusom and Jens Abildskov, 2013, "A Modelling Framework for Conventional and Heat Integrated Distillation Columns", Proceedings of the 18th Nordic Process Control Workshop (NPCW18)
	Jason Price, Jakob K. Huusom, Mathias Nordblad, John M. Woodley, 2013, "Optimization of Substrate Feeding for Enzymatic Biodiesel Production", Proceedings of the 18th Nordic Process Control Workshop (NPCW18)
	J. K. H. Knudsen, J. K. Huusom, J. B. Jørgensen, 2013, "Practical Implementations of Advanced Process Control for Linear Systems", Proceedings of the 18th Nordic Process Control Workshop (NPCW18)
	A.K. Vangsgaard, M. Mauricio-Iglesias, K.V. Gernaey, G. Sin, 2013, "Control of a Biological Nitrogen Removal Process in an Intensified Single Reactor Configuration", Proceedings of the 18th Nordic Process Control Workshop (NPCW18)

	F - Conference Presentations 2013
2013-01 Oral	Peam Cheali, Alberto Quaglia, Krist V. Gernaey and Gürkan Sin, 2013, "Synthesis and Design of Thermochemical and Biochemical Biomass Processing Networks under Uncertainty", European Congress of Chemical Engineering (ECCE-9), The Hague, The Netherlands, 20-25 April
2013-02 Poster	Nor Alafiza Yunus, Krist V. Gernaey, John M. Woodley and Rafiqul Gani, 2013, "Systematic Design of Tailor-Made Blended Products", European Congress of Chemical Engineering (ECCE-9), The Hague, The Netherlands, 20-25 April
2013-03 Poster	Mauricio-Iglesias, Miguel; Sin, Gürkan, 2013, "A model-based framework for incremental scale-up of wastewater treatment processes", European Congress of Chemical Engineering (ECCE-9), The Hague, The Netherlands, 20-25 April
2013-04 Poster	Mauricio-Iglesias, M.; Valverde-Pérez, B.; Sin, G., 2013, "Selection of controlled variables in bioprocesses. Application to a SHARON-Anammox process for autotrophic nitrogen removal", European Congress of Chemical Engineering (ECCE-9), The Hague, The Netherlands, 20-25 April
2013-05 Oral	Marina Fedorova, Gürkan Sin, Rafiqul Gani, 2013, "Computer-Aided Modeling Framework – A Generic Template as a Modeling Tool", European Congress of Chemical Engineering (ECCE-9), The Hague, The Netherlands, 20-25 April
2013-06 Oral	Larissa P. Cunico, Roberta Ceriani, Bent Sarup, Rafiqul Gani, 2013, "Modelling of physical and thermodynamic properties in systems containing edible oils and biodiesel", European Congress of Chemical Engineering (ECCE-9), The Hague, The Netherlands, 20-25 April
2013-07 Oral	A. Quaglia, G. Sin, R. Gani, 2013, "Efficient Information and Data Management in Synthesis and Design of Processing Networks", European Congress of Chemical Engineering (ECCE-9), The Hague, The Netherlands, 20-25 April
2013-08 Poster	Deenesh K. Babi, John M. Woodley, Rafiqul Gani, Don H. Jones, Arend J. Zeeuw, 2013, "Sustainable Intensified Process Retrofit for the Production of MDI", European Congress of Chemical Engineering (ECCE-9), The Hague, The Netherlands, 20-25 April
2013-09 Oral	Michele Mattei, Peter Krogh, Bo Depner, Georgios M. Kontogeorgis and Rafiqul Gani, 2013, "Design of a Tank Cleaning Blend through a Systematic Emulsified Product Design Methodology", European Congress of Chemical Engineering (ECCE-9), The Hague, The Netherlands, 20-25 April
2013-10 Oral	Rafiqul Gani, 2013, "Selection and design of solvents", 23rd Croatian Meeting of Chemists and Chemical Engineers, Osijek, Croatia, 22-24 April, **Plenary Lecture**
2013-11 Oral	Hande Bozkurt, Alberto Quaglia, Krist V. Gernaey, Gürkan Sin, 2013, "Design of future municipal wastewater treatment plants: A mathematical approach to manage complexity and identify optimal solutions", Asset management for enhancing energy efficiency in water and wastewater system, International Water Association, Marbella, Spain, 24-26 April
2013-12 Oral	Alberto Quaglia, Alessandra Pennati, Hande Bozkurt, Gürkan Sin, Rafiqul Gani, 2013, "A Tool to Support Optimal Industrial Wastewater Treatment Design and Analysis", Asset management for enhancing energy efficiency in water and wastewater system, International Water Association, Marbella, Spain, 24-26 April
2013-13 Oral	Niels Jensen, Sten Bay Jørgensen, 2013, "Learning Safety Assessment from Accidents in a University Environment", Presented at 14th EFCE Symposium on Loss Prevention and Safety Promotion in the Process Industries, Florence, Italy, 12-15 May

2013-14 Poster	Amol S. Hukkerikar, Bent Sarup, Gürkan Sin,and Rafiqul Gani, 2013, "Molecular structure based property modeling: Development/ improvement of property models through a systematic property-data-model analysis", PPEPPD-2013, Puerto Iguzaú, Argentina, 25-30 May
2013-15 Poster	Larissa P. Cunico, Roberta Ceriani, Bent Sarup, John O'Connell, Rafiqul Gani, 2013, "Data, analysis, modeling, and prediction of properties and phase equilibria for process design of edible oil and biodiesel systems", PPEPPD-2013, Puerto Iguzaú, Argentina, 25-30 May
2013-16 Poster	Michele Mattei, Georgios M. Kontogeorgis and Rafiqul Gani, 2013, "Development of a New Comprehensive Framework for Surfactant Selection and Design for Emulsion-based Chemical Product Design", PPEPPD-2013, Puerto Iguzaú, Argentina, 25-30 May
2013-17	Peam Cheali, Krist V. Gernaey, Gürkan Sin, 2013, "A computer-aided support tool for synthesis and design of biorefinery networks under uncertainty", The 3rd International Conference on Sustainable Chemical Product and Process Engineering (SCPPE 2013), Dalian, China, 27-30 May
2013-18	R. Gani, 2013, "Achieving sustainability through process intensification", The 3rd International Conference on Sustainable Chemical Product and Process Engineering (SCPPE 2013), Dalian, China, 27-30 May, **Plenary**
2013-19 Poster	A. Gizem Mutlu, A. Katrine Vangsgaard, Chen Lv, Carlos Domingo Félez, Gürkan Sin, Barth F. Smets, 2013, "Driving towards stratified aggregation in single-stage nitritation/anammox reactors by varying aeration regimes", IWA 9th international Conference on Biofilm Reactors, Paris, France, 28-31 May, **Poster Award**
2013-20 Poster	Peam Cheali, Krist V. Gernaey and Gürkan Sin, 2013, "Synthesis and design of optimal biorefinery using an expanded network with thermochemical and biochemical biomass conversion platforms", ESCAPE 23 June 9-12, 2013, Lappeenranta, Finland
2013-21 Oral	Nor Alafiza Yunus, Krist V. Gernaey, John M. Woodley and Rafiqul Gani, 2013, "Design of Sustainable Blended Products using an Integrated Methodology", ESCAPE 23 June 9-12, 2013, Lappeenranta, Finland
2013-22 Poster	Marina Fedorova, Gurkan Sin, Rafiqul Gani, 2013, "Computer-aided modeling framework – a generic modeling template", ESCAPE 23, Lappeenranta, Finland, 9-12 June
2013-23 Oral	Anna Katrine Vangsgaard, Miguel Mauricio-Iglesias, Krist V. Gernaey, Barth F. Smets, Gürkan Sin, 2013, "Control of a Biological Nitrogen Removal Process in an Intensified Single Reactor Configuration", ESCAPE 23, Lappeenranta, Finland, 9-12 June
2013-24	Alberto Quaglia, Bent Sarup, Gürkan Sin, Rafiqul Gani, 2013, "Design of a Generic and Flexible Data Structure for Efficient Formulation of Large Scale Network Problems", ESCAPE 23, Lappeenranta, Finland, 9-12 June
2013-25 Poster	Michele Mattei, Michael Hill, Georgios M. Kontogeorgis, Rafiqul Gani, 2013, "Design of an Emulsion-based Personal Detergent through a Model-based Chemical Product Design Methodology", ESCAPE 23, Lappeenranta, Finland, 9-12 June
2013-26 Poster	Thomas Bisgaard, Jakob Kjøbsted Huusom, Jens Abildskov, 2013, "Dynamic effects of diabatization in distillation columns", ESCAPE 23, Lappeenranta, Finland, 9-12 June
2013-27 Oral	Remus Mihail Prunescu, Jakob Munch Jensen, Mogens Blanke and Gürkan Sin, 2013, "Modelling and L1 Adaptive Control of pH in Bioethanol Enzymatic Process", 2013 American Control Conference (ACC) , Washington, DC, USA, 17-19 June, **Best Presentation in Session Award**
2013-28 Oral	Jing Wu, Laibin Zhang, Morten Lind, Wei Liang, Jinqiu Hu, Sten Bay Jørgensen, Gürkan Sin, Zia Ullah Khokhar, 2013, "Hazard Identification of the Offshore Three-phase Separation Process Based on Multilevel Flow Modeling and HAZOP", The 26th International Conference on Industrial, Engineering & Other Applications of Applied Intelligent Systems (IEA/AIE), Amsterdam, The Netherlands, 17-21 June

2013-29 Oral	Sawitree Kalakul, Pomthong Malakul, Kitipat Siemanond, and Rafiqul Gani, 2013, "Software Integration of Life Cycle Assessment and Economic Analysis for Process Evaluation", 6th International Conference on Process Systems Engineering, (PSE ASIA), Kuala Lumpur, Malaysia, 25-27 June
2013-30 Oral	S. Mangnimit, P. Malakul , R. Gani, 2013, "Sustainable Process Design of Biofuels: Bioethanol Production from Cassava rhizome", 6th International Conference on Process Systems Engineering, (PSE ASIA), Kuala Lumpur, Malaysia, 25-27 June
2013-31 Poster	Nor Alafiza Yunus, Krist V. Gernaey, John M. Woodley, Rafiqul Gani, 2013, "Systematic Design of Tailor-Made Blended Products", 6th International Conference on Process Systems Engineering, (PSE ASIA), Kuala Lumpur, Malaysia, 25-27 June
2013-32 Oral	Nor Alafiza Yunus, Krist V. Gernaey, John M. Woodley, Rafiqul Gani, 2013, "Model-Based Blend Design: Application to Lubricant Oils", 6th International Conference on Process Systems Engineering, (PSE ASIA), Kuala Lumpur, Malaysia, 25-27 June
2013-33 Oral	Noor Asma Fazli Abdul Samad, Gürkan Sin, Krist V. Gernaey, and Rafiqul Gani, 2013, "Uncertainty and Sensitivity Analysis on PAT System Performance for Crystallization Processes", 6th International Conference on Process Systems Engineering, (PSE ASIA), Kuala Lumpur, Malaysia, 25-27 June
2013-34 Oral	Rafiqul Gani, Deenesh K. Babi, Seyed Soheil Mansouri, Muhammad Imran Ismail, Jakob K. Huusom, John M. Woodley, 2013, "Achieving More Sustainable Solutions Through Process Intensification", 3rd International Congress on Sustainability Science & Engineering (ICOSSE), Cincinnati, OH, USA, 11-15 August, **Invited Keynote**
2013-35 Oral	Mauricio-Iglesias, Miguel; Sin, Gürkan, 2013, "Accelerating Scale-up of Bioprocesses using a Model-based and Multi-objective Optimisation Methodology", WCCE9 & APCChE 2013, Coex, Seoul, South Korea, 18-23 August
2013-36 Poster	A. K. Vangsgaard, M. Mauricio-Iglesias, K.V. Gernaey and G. Sin, 2013, "Control of a Novel Energy Efficient Biological Nitrogen Removal Process", WCCE9 & APCChE 2013, Coex, Seoul, South Korea, 18-23 August
2013-37 Poster	Saranya Mangnimit, Pomthong Malakul, and Rafiqul Gani, 2013, "Sustainable Process Design of Lignocellulose based Biofuel", WCCE9 & APCChE 2013, Coex, Seoul, South Korea, 18-23 August
2013-38 Oral	Igor Mitrofanov, Gurkan Sin, Rafiqul Gani, 2013, "PSE For Solvent Applications: A Generic Computer-aided Solvent Selection and Design Framework", WCCE9 & APCChE 2013, Coex, Seoul, South Korea, 18-23 August, **Invited Keynote**
2013-39 Poster	Sawitree Kalakul, Pomthong Malakul, Kitipat Siemanond, Rafiqul Gani, 2013, "A Generic Life Cycle Assessment Tool for Chemical-biochemical Processes", WCCE9 & APCChE 2013, Coex, Seoul, Korea, 18-23 August
2013-40 Oral	Rafiqul Gani, 2013, "Industry-academia Collaboration through the CAPEC Industrial Consortium", WCCE9 & APCChE 2013, Coex, Seoul, Korea, 18-23 August, **Invited Keynote**
2013-41 Oral	Rafiqul Gani, 2013, "A process Systems Engineering Approach for Managing the Complexity in Chemical Product-Process", WCCE9 & APCChE 2013, Coex, Seoul, Korea, 18-23 August, **Invited Keynote**
2013-42 Oral	Jason Price, Jakob K. Huusom, Mathias Nordblad, John M. Woodley, 2013, "Optimization of Substrate Feeding for Enzymatic Biodiesel Production", 18th Nordic Process Control Workshop (NPCW18), Oulu, Finland, 20-23 August
2013-43 Oral	J. K. H. Knudsen, J. K. Huusom, J. B. Jørgensen, 2013, "Practical Implementations of Advanced Process Control for Linear Systems", 18th Nordic Process Control Workshop (NPCW18), Oulu, Finland, 20-23 August

2013-44 Poster	Thomas Bisgaard, Jakob Kjøbsted Huusom and Jens Abildskov , 2013, "A Modelling Framework for Conventional and Heat Integrated Distillation Columns", 18th Nordic Process Control Workshop (NPCW18), Oulu, Finland, 20-23 August
2013-45 Oral	A.K. Vangsgaard, M. Mauricio-Iglesias, K.V. Gernaey, G. Sin, 2013, "Control of a Biological Nitrogen Removal Process in an Intensified Single Reactor Configuration", 18th Nordic Process Control Workshop (NPCW18), Oulu, Finland, 20-23 August
2013-46 Oral	Noor Asma Fazli Abdul Samad, Kresten Troelstrup Meisler, Gürkan Sin, Krist V. Gernaey, Rafiqul Gani, 2013, "A Systematic Framework for Design of Process Monitoring and Control (PAT) Systems for Crystallization Processes", 20th International Workshop on Industrial Crystallization (BIWIC2013), Odense, Denmark, 18-20 September
2013-47 Poster	Kresten T. Meisler, Nicolas von Solms, Krist V. Gernaey, Rafiqul Gani, 2013, "Crystallization Kinetics within a Generic Modelling Framework", 20th International Workshop on Industrial Crystallization (BIWIC2013), Odense, Denmark, 18-20 September
2013-48 Poster	A.K. Vangsgaard, M. Mauricio-Iglesias, A.G. Mutlu, K.V. Gernaey, B.F. Smets and G. Sin, 2013, "Performance of an autotrophic nitrogen removing reactor: Diagnosis through fuzzy logic", 11th IWA conference on instrumentation control and automation (ICA), 18-20 September 2013, Narbonne, France
2013-49 Poster	H. Bozkurt, A. Quaglia , K.V. Gernaey and G. Sin, 2013, "Superstructure development and optimization for design/retrofit of municipal wastewater treatment plants",11th IWA conference on instrumentation control and automation (ICA), Narbonne, France, 18-20 September
2013-50 Oral	Montero-Castro, Ignacio; Mauricio-Iglesias, Miguel; Mollerup, Ane L.; Sin, Gürkan, 2013, "Self-optimising control of sewer systems", 11th IWA conference on instrumentation control and automation (ICA), Narbonne, France, 18-20 September
2013-51 Oral	Rafiqul Gani, 2013, "Chemical Engineering Education, Research & Development in Europe", The 20th Anniversary Celebration, Department of Chemical and Biomolecular Engineering, The Hong Kong University of Science and Technology, Hong Kong, 5 October, **Plenary Lecture**
2013-52 Oral	Rafiqul Gani, 2013, "Managing the Complexity in Chemical Product Engineering", XIVe Congrès de la Société Française de Génie des Procédés (SFGP 2013), Lyon, France, 8 October, **Plenary Lecture**
2013-53 Oral	Michele Mattei, Georgios M. Kontogeorgis and Rafiqul Gani , 2013, "Predicting Surfactant-related Properties for Chemical-based Product Design", AIChE 2013, San Francisco, USA, 3-8 November
2013-54 Oral	Michele Mattei, Georgios M. Kontogeorgis and Rafiqul Gani, 2013, "Use of Water-Oil-Surfactant System Phase Behavior Data/Model for Emulsion-based Chemical Product Design", AIChE 2013, San Francisco, USA, 3-8 November
2013-55 Oral	Deenesh K. Babi, Johannes Holtbruegge, Philip Lutze, John M. Woodley, Andrzej Górak, Rafiqul Gani, 2013, "A Framework for Process Synthesis integrated with Sustainability and Process Intensification", AIChE 2013, San Francisco, USA, 3-8 November
2013-56 Oral	Rafiqul Gani, 2013, "An Intelligent System for Modelling, Design and Analysis of Chemical Processes", AIChE 2013, San Francisco, USA, 3-8 November
2013-57 Oral	Kresten Troelstrup Meisler, Noor Asma Fazli Abdul Samad, Krist V. Gernaey and Rafiqul Gani, 2013, "Generic Modelling Framework for Design and Analysis of Crystallization Operations", AIChE 2013, San Francisco, USA, 3-8 November
2013-58 Oral	Alberto Quaglia, A. Anantpinijwatna, G. Sin, R. Gani, 2013, "An Ontology for Information and Data Management for Synthesis and Design of Processing Networks", AIChE 2013, San Francisco, USA, 3-8 November

2013-59 Oral	Kresten Troelstrup Meisler, Krist V. Gernaey, Nicolas von Solms, Rafiqul Gani and Zoltan K. Nagy, 2013, "Study of Crystallization Kinetics Within a Generic Modelling Framework", AIChE 2013, San Francisco, USA, 3-8 November
2013-60 Oral	Muhammad Rizwan, Jay H. Lee and Rafiqul Gani, 2013, "Optimal Design of Microalgal Biomass Processing Network", AIChE 2013, San Francisco, USA, 3-8 November
2013-61 Oral	John P. O'Connell and Rafiqul Gani, 2013, "Capec Consortium: Effective Academic-Industrial Interactions Strengthened By Surveys and Analyses of Gaps in Properties Modeling", AIChE 2013, San Francisco, USA, 3-8 November
2013-62 Oral	Peam Cheali, Krist V. Gernaey and Gürkan Sin, 2013, "Synthesis and Design of Biorefinery Processing Networks with Uncertainty and Sustainability analysis", AIChE 2013, San Francisco, USA, 3-8 November
2013-63 Oral	Jason Price, Mathias Nordblad, John M. Woodley, Jakob K. Huusom, 2013, "Optimization of Substrate Feeding for Enzymatic Biodiesel Production", AIChE 2013, San Francisco, USA, 3-8 November
2013-64 Poster	Seyed S. Mansouri, Muhammad I. Ismail, Deenesh K. Babi, Jakob K. Huusom, Rafiqul Gani, 2013, "Sustainable and Intensified Design of a Biodiesel Production Process", AIChE 2013, San Francisco, USA, 3-8 November
2013-65 Poster	Alberto Quaglia, Gürkan Sin, Rafiqul Gani, 2013, "A Multi-Scale Framework for Enterprise-Wide Design and Retrofit of Processing Networks: From Meso- to Mega-Scale", AIChE 2013, San Francisco, USA, 3-8 November
2013-66 Oral	Remus Mihail Prunescu, Mogens Blanke and Gürkan Sin, 2013, "Modelling and L1 Adaptive Control of Temperature in Biomass Pretreatment", 52nd IEEE Conference on Decision and Control, Firenze, Italy, 10-13 December
2013-67 Poster	Mauricio-Iglesias, M.; Vangsgaard, A.K.; Gernaey, K; Sin, G., 2013, "A fuzzy-logic based diagnosis and control of a reactor performing complete autotrophic nitrogen removal", 12th IFAC Symposium on Computer Applications in Biotechnology (CAB 2013), Mumbai, India, 16-18 December
2013-68 Oral	Jason Price, Mathias Nordblad, John M. Woodley, Jakob K. Huusom, 2013, "Application of Uncertainty and Sensitivity Analysis to a Kinetic Model for Enzymatic Biodiesel Production", 12th IFAC Symposium on Computer Applications in Biotechnology (CAB 2013), Mumbai, India, 16-18 December
2013-69 Poster	Mauricio-Iglesias, M. Montero-Castro, I. Mollerup, A.L. Sin, G., 2013, "Self-optimising control of sewer systems", 10th International IFAC Symposium on Dynamics and Control of Process Systems (DYCOPS 2013), Mumbai, India, 18-20 December, **Best Poster Award**
2013-70 Poster	Thomas Bisgaard, Jakob Kjøbsted Huusom and Jens Abildskov, 2013, "A Modeling Framework for Conventional and Heat Integrated Distillation Columns", 10th International IFAC Symposium on Dynamics and Control of Process Systems (DYCOPS 2013), Mumbai, India, 18-20 December, **Best Poster Award**
2013-71 Oral	Muhammad Rizwan, Jay H. Lee, Rafiqul Gani, 2013, "Superstructure optimization of biodiesel production from microalgal biomass", 10th International IFAC Symposium on Dynamics and Control of Process Systems (DYCOPS 2013), Mumbai, India, 18-20 December

	F - Conference Presentations 2014

2014-01 Poster	Hande Bozkurt, Alberto Quaglia, Krist V. Gernaey and Gürkan Sin, 2014, "Early-stage design of municipal wastewater treatment plants – presentation and discussion of an optimization based concept", 4th IWA/WEF Wastewater treatment modelling seminar (WWTMod 2014), Spa, Belgium, 30 March - 2 April
2014-02	Jason Price, Mathias Nordblad, John M. Woodley, Jakob K. Huusom, 2014, "Mechanistic Modelling Of Enzymatic Biodiesel Production For Fed Batch Control", 3rd European Conference on Process Analytics and Control Technology (EuroPACT 2014), Barcelona, Spain, 6-9 May
2014-03 Oral	Rafiqul Gani, 2014, "A framework for achieving more sustainable process synthesis-designs", 2014 CAS-TWAS Symposium on Advanced Engineering Science for Sustainable Development (AES2014), Beijing, China, 28-30 May, **Plenary Lecture**
2014-14 Oral	Rafiqul Gani, 2014, "A computer aided framework for multiscale modeling", Global Predictive Modeling Network Workshop "Enabling Multi-scale Modeling in Syngenta", Syngenta, RTD, North Carolina, USA, 3-5 June, **Invited Lecture**
2014-05	Alberto Quaglia, Gürkan Sin, Rafiqul Gani, 2014, "Financial risk analysis in the synthesis and design of processing networks: Balancing risk and return", European Symposium on Computer Aided Process Engineering (ESCAPE 24), Budapest Hungary, 15-18 June, **Keynote lecture**
2014-06	Michele Mattei, Nor A. Yunus, Sawitree Kalakul, Georgios M. Kontogeorgis, John M. Woodley, Krist V. Gernaey, Rafiqul Gani, 2014, "The Virtual Product-Process Design Laboratory for Structured Chemical Product Design and Analysis", European Symposium on Computer Aided Process Engineering (ESCAPE 24), Budapest Hungary, 15-18 June
2014-07 Oral	Hande Bozkurt, Alberto Quaglia, Krist V. Gernaey and Gürkan Sin, 2014, "Superstructure development and optimization under uncertainty for design and retrofit of municipal wastewater treatment plants", European Symposium on Computer Aided Process Engineering (ESCAPE 24), Budapest Hungary, 15-18 June
2014-08	Carina L. Gargalo, Ana Carvalho, Henrique A. Matos, Rafiqul Gani, 2014, "Techno-Economic, Sustainability & Environmental Impact Diagnosis (TESED) Framework", European Symposium on Computer Aided Process Engineering (ESCAPE 24), Budapest Hungary, 15-18 June
2014-09	Marina Fedorova, Gürkan Sin, Rafiqul Gani, 2014, "Computer-Aided Template for Model Reuse, Development and Maintenance", European Symposium on Computer Aided Process Engineering (ESCAPE 24), Budapest Hungary, 15-18 June
2014-10	D. K. Babi, J. M. Woodley, R. Gani, 2014, "Achieving More Sustainable Designs through a Process Synthesis-Intensification Framework", European Symposium on Computer Aided Process Engineering (ESCAPE 24), Budapest Hungary, 15-18 June
2014-11 Oral	P. Cheali, A. Quaglia, K. V. Gernaey, G. Sin, 2014, "Uncertainty Analysis in Raw Material and Utility Cost of Biorefinery Synthesis and Design", European Symposium on Computer Aided Process Engineering (ESCAPE 24), Budapest Hungary, 15-18 June

	G – Invited Seminars 2013
	Rafiqul Gani, 2013, "Computer Aided Solvent Selection, Design and Analysis", Bayer Lecture, Carnegie Mellon University, Pittsburgh, PA, USA, 5 March
	Rafiqul Gani, 2013, "Industry-academia collaboration through the CAPEC industrial consortium", Pfizer, Hartford, CT, USA, 7 March
	Rafiqul Gani 2013, "Achieving More Sustainable Solutions through Process Intensification", The 50th Anniversary Symposium of the Department of Chemical & Biological Engineering, Korea University, South Korea, 21 August

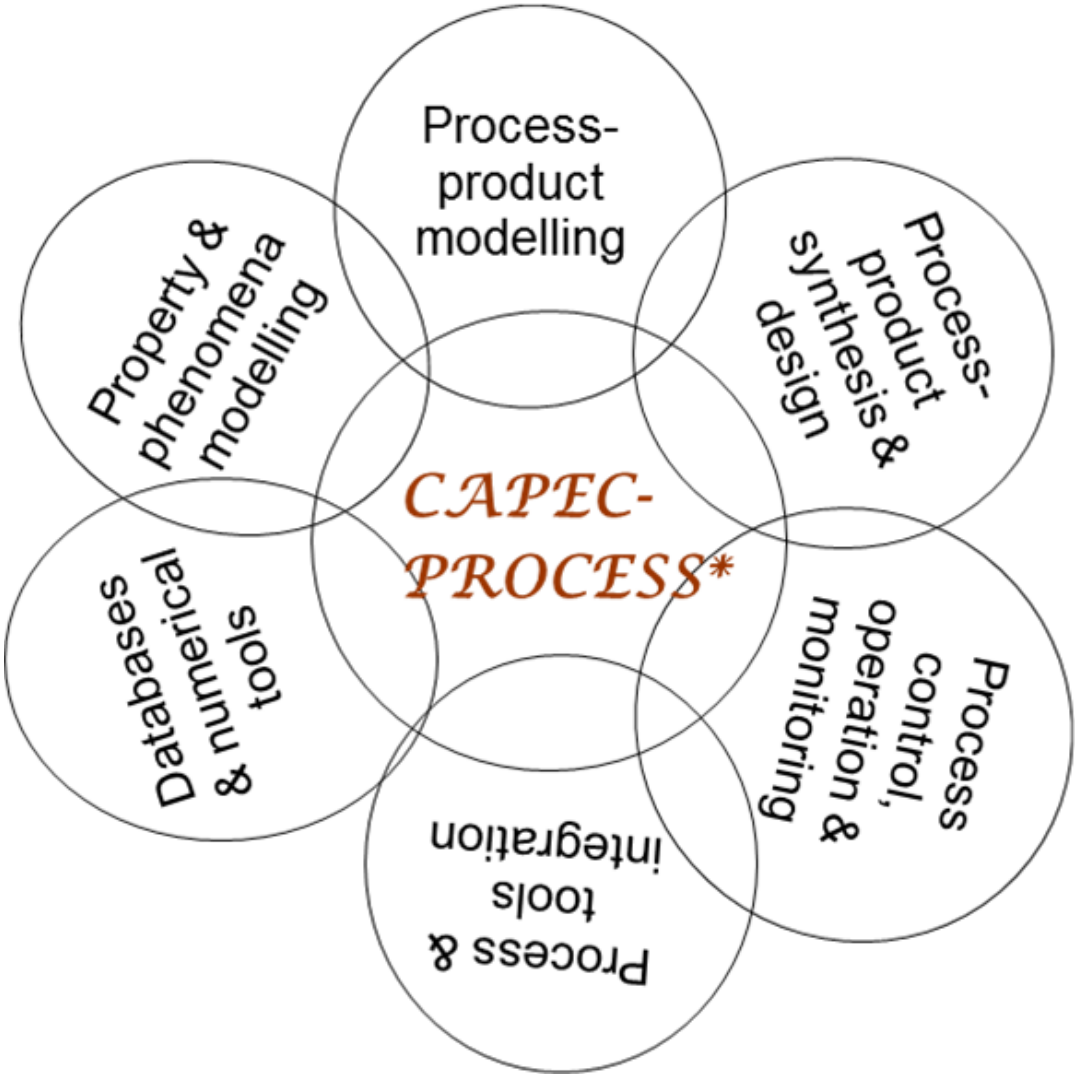
	Rafiqul Gani 2013, “Model based methods and tools for process systems engineering”, Post WCCE’09 Conference: Frontiers in Multiscale Systems Engineering, KAIST Department of Chemical & Biomolecular Engineering, KAIST University, South Korea, 24 August
	Gürkan Sin, 2013, “Early stage design and analysis of biorefinery networks”, Safety & Environmental Technology group at the Institute for Chemical and Bio-Engineering, ETH Zürich, Switzerland, 25 October
	Rafiqul Gani, 2013, "A New Paradigm for Chemical Engineering?", the ORYX GTL seminar series in chemical engineering at the Texas A&M University, Qatar, Doha, 27 November

	G – Invited Seminars 2014
	Rafiqul Gani, 2014, “Managing the Complexity in Chemical Product Engineering”, Tsinghua University, Beijing, China, 26 February
	Rafiqul Gani, 2014, “Achieving more sustainable solutions through process intensification”, IPE, Beijing, China, 28 February
	Rafiqul Gani, 2014, “Achieving more sustainable solutions through process intensification”, Northwestern University, Departmental Seminar, Chicago, USA, 17 April
	Rafiqul Gani, 2014, “Managing the Complexity in Chemical Product Engineering”, Northwestern University, Chicago, USA, 18 April
	Rafiqul Gani, 2014, “A new paradigm for chemical engineering?”, Tsinghua University, Beijing, China, 30 May
	Rafiqul Gani, 2014, ”Achieving more sustainable solutions through process intensifications”, Tianjin University, Tianjin, China, 24 May
	Rafiqul Gani, 2014, ”Overview of CAPEC and ICAS”, SINOPEC, Beijing, China, 26 May

	Accepted/planned conference presentations 2014
Oral	H. Bozkurt, A. Quaglia, K.V. Gernaey and G. Sin, 2014, “An optimization Based Framework for Design and Retrofit of Municipal Wastewater Treatment Plants: Case study on side-stream nitrogen removal technologies”, 2nd IWA Specialized International Conference “Ecotechnologies for Wastewater Treatment (EcoSTP2014), Verona, Italy, 23-25 June
	Rafiqul Gani, Ka M. Ng, 2014, ”Product Design - From Molecules to Formulations to Devices”, 8th International Conference on Foundations of Computer-Aided Process Design (FOCAPD 2014), Cle Elum, Washington, USA, 13-17 July, **Invited Keynote Lecture**
	Marina Fedorova, Emmanouil Papadakis, Kresten T. Meisler, Gürkan Sin, Rafiqul Gani, 2014, “Application of the Generic Modeling Template Approach to Unsaturated Fatty Acid Oxidation and Crystallization Systems”, 8th International Conference on Foundations of Computer-Aided Process Design (FOCAPD 2014), Cle Elum, Washington, USA, 13-17 July
	Amata Anantpinijwatna, Gürkan Sin, John P. O’Connell, Rafiqul Gani, 2014, “A Framework for the Modelling of Biphasic Reacting Systems”, 8th International Conference on Foundations of Computer-Aided Process Design (FOCAPD 2014), Cle Elum, Washington, USA, 13-17 July
	Daniela de Faria, Alberto Quaglia, Fernando Pessoa, Rafiqul Gani, 2014, “Early Stage Design of a Biorefinery from Castor Oil”, 8th International Conference on Foundations of Computer-Aided Process Design (FOCAPD 2014), Cle Elum, Washington, USA, 13-17 July

	Deenesh K. Babi, Johannes Holtbruegge, Philip Lutze, Andrzej Górak, John M. Woodley, Rafiqul Gani, 2014, "Sustainable Process Synthesis-Intensification", 8th International Conference on Foundations of Computer-Aided Process Design (FOCAPD 2014), Cle Elum, Washington, USA, 13-17 July
	Jakob K Huusom, 2014, "Integration of Design and Control", 8th International Conference on Foundations of Computer-Aided Process Design (FOCAPD 2014), Cle Elum, Washington, USA, 13-17 July, **Invited Lecture**
	P. Cheali, A. Quaglia, K. V. Gernaey, G. Sin, 2014, "Synthesis and design of hybrid biorefinery systems a structural optimisation approach and uncertainty analysis", 21st International Congress of Chemical and Process Engineering (CHISA 2014), Prague, Czech Republic, 23-27 August
	Z. B. Handani, A. Quaglia, G. Sin, R. Gani, 2014, "An integrated approach for synthesis and design of process and water/wastewater networks", 21st International Congress of Chemical and Process Engineering (CHISA 2014), Prague, Czech Republic, 23-27 August
	Jakob Kjøbsted Huusom og John Bagterp Jørgensen., 2014, "A Realistic Process Example for MIMO MPC based on Autoregressive Models", Proceedings of 19th World Congress of the International Federation of Automatic Control (IFAC'14), Cape Town, South Africa, 24-29 August
	Jason Price, Mathias Nordblad, John M. Woodley, Jakob K. Huusom, 2014, "Fed-Batch Feeding Strategies for Enzymatic Biodiesel Production", 19th World Congress of the International Federation of Automatic Control (IFAC'14), Cape Town, South Africa, 24-29 August
	P. Lützen, M. Mauricio-Iglesias, J.K. Huusom, J. Abildskov, 2014, "Control benchmark for solvent recovery by distillation", 10th International Conference on Distillation & Absorption 2014, Friedrichshafen, Germany, 14-17 September
	J. Abildskov, J.P. O'Connell, 2014, "Azeotropic pressure sensitivity modeling", 10th International Conference on Distillation & Absorption 2014, Friedrichshafen, Germany, 14-17 September
	K. Meyer, L. Ianiaciello, J.E. Nielsen, T. Bisgaard, J.K. Huusom, J. Abildskov, 2014, "HIDiC - Design, sensitivity and graphical representation", 10th International Conference on Distillation & Absorption 2014, Friedrichshafen, Germany, 14-17 September
	M. Mauricio-Iglesias, T. Bisgaard, J. Abildskov, H. Kristensen, K.V. Gernaey, J.K. Huusom, 2014, "Model-based benchmark of pressure control structures in distillation columns", 10th International Conference on Distillation & Absorption 2014, Friedrichshafen, Germany, 14-17 September
	M. Mauricio-Iglesias, J. Abildskov, K.V. Gernaey, V. Vahedi, J.K. Huusom, 2014, "Optimisation of energy consumption in ethanol recovery. Focus on trace compounds removal", 10th International Conference on Distillation & Absorption 2014, Friedrichshafen, Germany, 14-17 September
	T. Bisgaard, J.K. Huusom, Jens Abildskov, 2014, "Impact on Model Uncertainty of Diabatization in Distillation Columns", 10th International Conference on Distillation & Absorption 2014, Friedrichshafen, Germany, 14-17 September

7.4 CAPEC-PROCESS Consortium Members



*** Systematic methods and tool**

Please contact Mrs. Eva Mikkelsen (eva@kt.dtu.dk) for further information