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CAPEC-PROCESS Research Report 2013

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PEC13-25

CAPEC-PROCESS Industrial Consortium
Research Report – 2013

Rafiqul Gani& John M. Woodley

June 2013

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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 2012 to June 2013. 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 centersare 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 an equal number of new projects have been started. More specifically, within CAPEC: Noor Asma Fazli bin Abdul Samad (PEC12-40) and Azizul Azri Bin Mustaffa (PEC12-60); within PROCESS: Rita Lancastre Fernandez; and, within PROCESS-CAPEC:Naweed Al-Haque (PEC13-35). Alberto Quaglia and Amol Hukkeriker from CAPEC are adding final touches to their PhD-theses to denfend later this year, and Joana Lima Ramos from PROCESS will defend her PhD-thesis on 19 June 2013. At the same time, new PhD-students (Zainatul B. Handani, Sawitree Kalakul, Søren Heintz, Rolf Hoffmeyer Ringborg, Anders Nørregaard, Hilde Larsson, Ines Pereira Rosinha)have started their PhD-projects at CAPEC and PROCESS centers while 4 new post-doctoral projects were also started (Noor Asma Fazli bin Abdul Samad, Rita Lancastre Fernandez, Miguel Mauricio Iglesias and Xavier Flores Alsina).

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 started projects with AstraZeneca andAlfa-Laval from our consortium members, and,Univ of Lorraine (France), ChulalongkornUniv-PPC (Thailand), PROSPECT-UTM (Malaysia), Univ of Kansas (USA), Univ of West Virginia (USA) and Auburn Univ (USA) from academia.

We would like to acknowledge the financial support in the form of membership fees from our member companies. We would like to welcome Welcron-Hantec(Korea) and Harper &Vedel(Denmark) as new consortium members. For funding of PhD and post-doctoral research projects we would like to thank the Danish funding agencies FTP, EFP and ATV and the EC-research programs under FP7. Also, we would like to thank the governments of Malaysia, Brazil and Thailand for sending students with PhD/MSc-scholarships.

Finally, we take this opportunity to thank all co-workers of CAPECand PROCESS for their hard work and dedication. The research results highlighted in this report are their achievements. This is the 16th year since CAPEC and the industrial consortium was established.At PROCESS, we are happy to announce that Krist V. Gernaey was appointed as full professor earlier this year – congratulations to Krist.

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 2013

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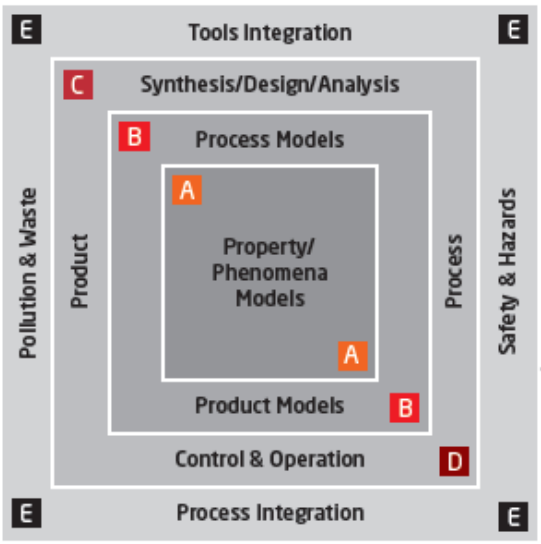
1. Introduction

1.1 The CAPEC Center

ResearchatCAPECisorganizedinterms ofsixresearchprograms(see*Fig1.1*).At theinnermostlevel(researchprograms A,B),thetopicsare relatedtofunda- mental researchwhileattheoutermost level(E),thetopicsare relatedtoapplied research.Intheintermediatelevels(C, D),systematicmodel-basedalgorithms, methodsand tools aredevelopedbyem- ployingtheresultsfromtheinnerlevels for useinapplied researchintheouter level.Sinceallresearchprogramsneed numericaltools anddatabases,research programFsuppliesthisneed toalllevels.



The main theme of the research at CAPEC is to manage the complexity in the systematic analysis and solution of a wide range of product-process engineering problems from various industrial sectors.

Figure 1.1: Organization of research in CAPECin 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 analysisequipments). 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 50 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.
- IEA-IETS: This is an EUDP funded project to support Danish participation in IEA-IETS for the period 2011-2013. This is about particiapting in International Energy Agency (IEA) implementing agreement on industrial energy related technologies and systems (IETS). CAPEC has received funding to coordinate a task group on Energy efficient separation 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.

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 industrial production 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 process validation. Two demonstration units operate in the pilot facilities (both for immobilized and soluble enzyme reactions at 10-20L scale). 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 eceonomic and environmental evaluation. The research is divided into 7 research areas:

Main research areas:

1. Micro 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 process screening tools.

2. Continuous processes – the development of new continuous or semi-continuous processes form batch. New concepts are developed including the creation of gereic process plant.

3. 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.

4. Process intensification and intensified unit operation – development of integrated unit operations (e.g. ISPR) and methods and tools for assessing new operations and processes operating at an intensified level.

5. Process Analytical Technologies (PAT) – development of monitoring and control techniques to allow on-line adjustment of process parameters such that product quality can be maintained. Particular focus is on the phramacutical industry (where the FDA drives such changes).

6. Scale translation – development of techniques for predicting scale-up and scale-down of processes and we as experimental validation.

7. Fermentation technology – development of scale-translation and modelling of fermentation process.

The PROCESS Center is involved in the following large collaborative projects in Denmark and in Europe:

- Towards Robust Fermentation Processes by Targeting Population Heterogeneity at Microscale is a project established in 2009 with the Danish Council for Strategic Research, DTU Systems Biology, DTU Fotonik, Department of Biology (University of Copenhagen), Department of Biotechnology, Chemistry and Environmental Engineering (Aalborg University), Crystal Fibre A/S, FermencoApS and Foss A/S. It is focused on characterization and control of the heterogeneity of a population of microorganisms in fermentation.
- In the pharmaceutical sector several projects (BIONEXGEN, AMBIOCAS and BIOTRANS) sustain the development of the next generation of enzyme based methods for the synthesis of optically pure molecules. These EC-funded projects are with many industrial and academic partners. The Center is also involved in a 5-year project with Lundbeck aiming at moving from batch towards continuous production, Specifically on the development of microbioreactors, PROCESS has initiated a project of the Free Research Council – Technology and Production Sciences (FTP) (Novel greener and lean processes using integrated microfactories).
- A new FP7 project (BIOINTENSE) has started 2012. It is focused on microscale approach for the rapid development of biocatalytic processes. PROCESS is the project coordinator. Other new EC-projects will be BIOOX and INTERACT.
- PROCESS has joined the SANITAS project, an EC-funded project (ITN) with focus on the development of next generation of modelling and simulation tools for performance evaluation of wastewater treatment plants.

The vision of the Center for Process Engineering and Technology is to provide the necessary support to enable the next-generation of industrial production processes to be implemented. 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.

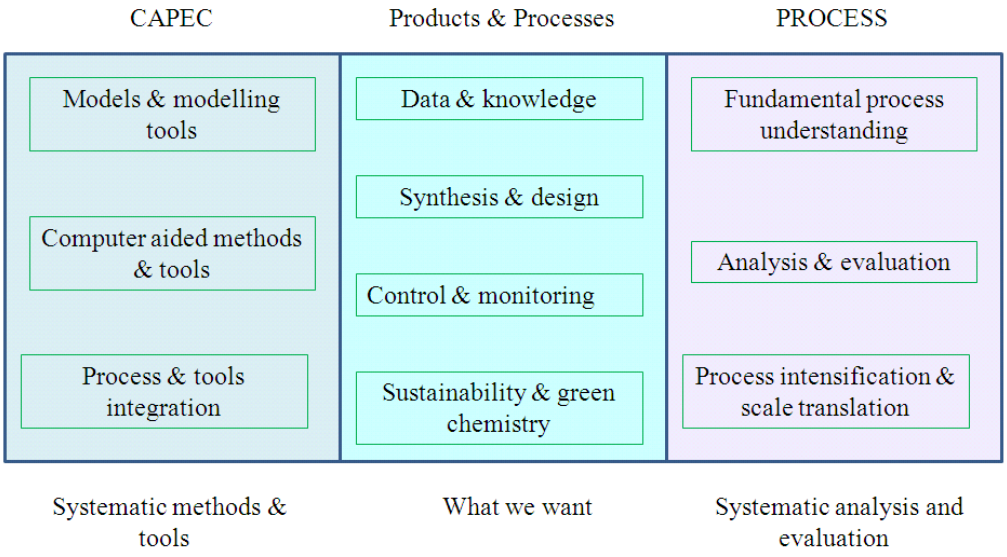


Figure 1.2: Collaboration between CAPEC and PROCESS centers

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.

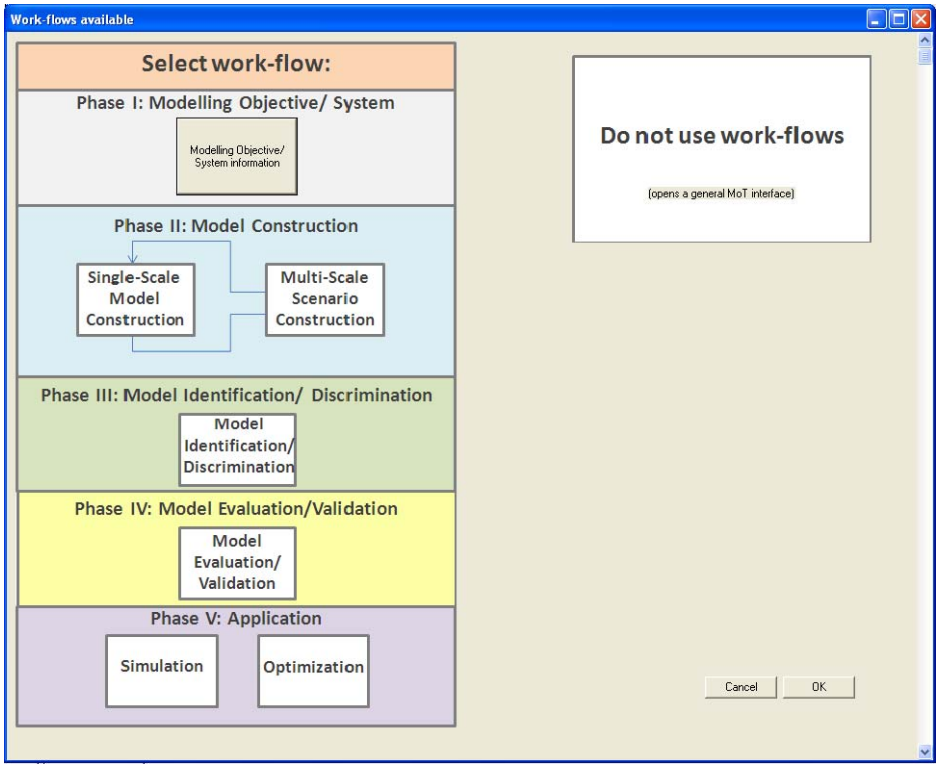


Figure 1.3: Representation of the computer aided modeling framework

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. From 1998 until 2005, Krist was employed as a postdoctoral fellow at Ghent University, ÉcolePolytechnique de Montréal, Quebec, Canada, DTU Chemical Engineering and Lund University, Sweden. 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. 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
- Development of sensors for on-line biomass characterization, for example via image cytometry
- 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

A 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. Several other PhD projects in this area will be started during the second half of 2013.

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 identifyprocess-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 CAPECand PROCESS are conducted by the faculty members of the two centerstogether 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.

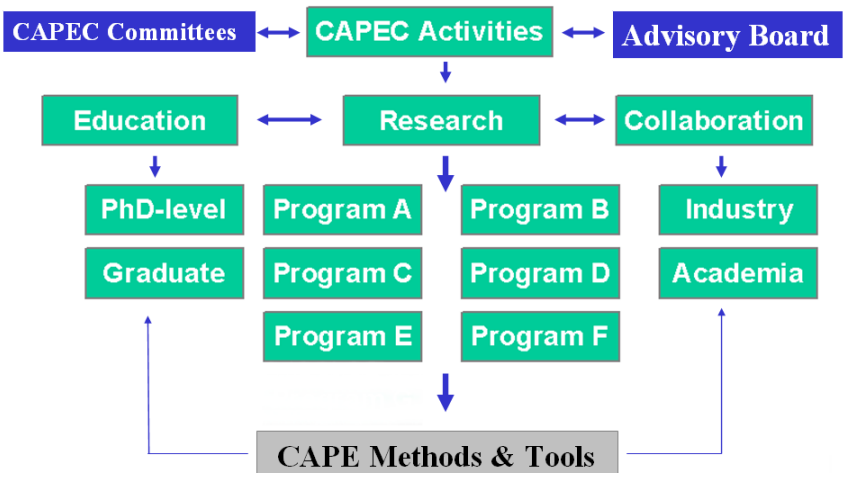


Figure 2.1: Organization of educational and research activities within CAPEC.

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*

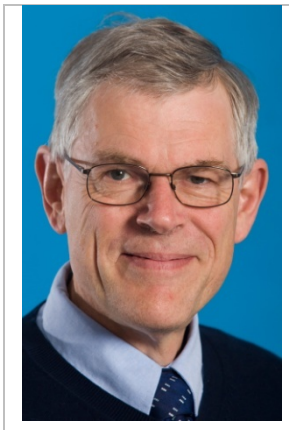
Associate Professor Gürkan Sin (GSI)

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
- 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 research covers process modelling; process design/analysis; process control, monitoring & operation; and, process integration-intensification. KVG is a faculty member of the PROCESS center. Currently active research topics are listed below. • Process modelling, applied to fermentation, biocatalysis, wastewater treatment, food production, pharmaceutical production, biorefineries; focus on the use of systems of ODEs, but increasingly also population balance models (PDEs) and CFD. • Parameter estimation and model analysis (*e.g.*, sensitivity and uncertainty analysis), *i.e.*, linking process models to plant data • Design of new reactor systems, including microbioreactors for enzymatic reactions and fermentation + systems for continuous production of pharmaceuticals • Design of PAT systems + biorefineries • On-line monitoring of fermentation processes + continuous organic synthesis, Process Analytical Technology (pharmaceutical production) • Benchmarking of control strategies for wastewater treatment plants ***Research Areas (PROCESS):*** *1-7*
 **Professor John Woodley (JW)**	JW is the head of the PROCESS center and his main research interests lie in the following topics: • Next generation processes (integration of biocatalysis with heterogeneous and homogeneous catalysis; processes based on renewable; green chemistry; pharmaceutical processes; and, biorefineries). • Methodology (process intensification; reactor design; evaluation methodologies) Applications in chemical, biochemical (e.g. biotechnology, fermentation technology, etc), pharmaceutical, food industries. ***Research areas (PROCESS):*** *1-7*

Associate Professor Ulrich Krühne (ULKR)

ULKR coordinates the microtechnological based research and development activities at the PROCESS enter. This research area has gained significant importance in chemical engineering andspecial topics of research interest are:

- Numerical and experimental investigation of micro scaled fluid dynamic properties and their influence on chemical, biochemical and physical interactions
- Integration of different miniaturized unit operations into a single step process
- Optimization of microscaled fluidic systems based on computational fluid dynamic (CFD) and kinetic models.

The research area is interactively connecting with the biocatalytic work and fermenation activities at the center.

Research areas (PROCESS): *1-7*

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
Noor Asma Fazli bin Abdul Samad	The rational selection of polymers for pharmaceutical formulations	RaG	10-2012	07-2013	Asta Zeneca

PROCESS Post-Doc	Project Title	Supervisors	Start	End	Funding
Rita Lencastre Fernandes	Challenges in extracting information from bioprocess industry data	KVG	03-2013	02-2014	BioPro
Miguel Mauricio Inglesias	Advanced tools for easy(ier) control	KVG	01-2013	12-2014	BioPro
Xavier Flores-Alsina	New PROcess models to simulaTE, benchmark and control Urban wastewater treatment Systems: the PROTEUS project	KVG	05-2013	04-2015	BioPro

CAPEC PhD Student	Project Title	Supervisors	Start	End	Funding
Azizul Azri Bin Mustaffa	Development and analysis of Group-Contribution^{plus} models for property prediction of organic chemical systems	RaG/GK	4-2009	2-2013	Government of Malaysia
Amol Hukkerikar	Model based integrated process-product design – retrofitting and optimisation	GSI/RaG Bent Sarup	6-2010	5-2013	Alfa Laval, MultiMod
Alberto Quaglia	Incremental refinement of process design	GSI/RaG/ Bent Sarup	6-2010	5-2013	MultiMod, Alfa Laval
Igor Mitrofanov	A methodology for systematic design and selection of green solvents for increased yield in organic reactions	RaG/GSI	11-2010	4-2013	MultiMod
Michele Mattei	Systematic methodology for design of	RaG/GK	8-2011	7-2014	DTU, CAPEC,

	emulsion based chemical products				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	8-2015	DTU
Zainatul Bahiyah BintiHandai	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/ Kontogeorgis	6-2013	5-2016	DTU; Alfa Laval; Qatar Fund
Andreas Åberg	Modeling and Operation of Diesel Engine Exhaust Gas Cleaning Systems	JKH/HaldorTopsøe	8-2013	7-2016	HTF/KT
AmataAnantpinijwatna	Generic model-based tailor-made design and analysis of biphasic reacting systems	RaG/GSI	8-2013	7-2016	Government of Thailand

CAPEC-PROCESS PhD Student	**Project Title**	**Supervisors**	**Start**	**End**	**Funding**
Noor Asma Fazli Bin Abdul Samad	Control of Process Operations and Monitoring of Product Qualities Through Hybrid Multi-Scale Model-Based Analysis	RaG/GSI/ KVG	1-2009	12-2012	Government of Malaysia
Naweed Al-Haque	Modelling controlled release of substrate and removal of product in biocatalysis	JW/RaG/PT	11-2009	5-1013	DTU/AMBIOCAS
Nor Alafiza Yunus	Tailor-made design of chemical products: Bio-fuels and other blended products	RaG/JW/ KVG	7-2010	11-2013	Government of Malaysia
Anna Katrine Vangsgaard	Modeling and Control of Novel Membrane Processes for Autotrophic Nitrogen Removal	GSI/ KVG/BFS	9-2010	8-2013	DSF EcoDesignMBR
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	Plantwidemodelling and control for N2O from WWTP	GSI/KVG	9-2013	8-2016	DSF

PROCESS PhD Student	**Project Title**	**Supervisor**	**Start**	**End**	**Funding**
Rui Xue	Reactor selection for multi-step enzymatic reactions	JW/AM/JDM	12-2010	11-2013	HMO/DTU
Jason Price	Optimization of substrate feeding for enzymatic biodiesel production	JW/JKH/MAN	09-2011	08-2014	Biodiesel/DTU
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
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 Pereira 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

External PhD-Students	Project Title	Supervisor	Start	End	Funding
Klaus Reinholdt Nyhuus Hansen	New Product Introduction for the Pharmaceutical Industry	MG/RaG	9-2009	8-2012	DTU Management
LidaSimasatitkul	From Biomass to Fatty Alcohol via Bio-Diesel: Optimal Process Design	Arpornwichanop /RaG	1-3-2011	(04-2013)	Chulalongkorn University, Thailand
Muhammad Zaman	Process Simulations Oriented Solvent Design for Carbon Dioxide Capture	RaG	1-2012	(12-2013)	KAIST, Korea
Muhammad Rizwan	Optimal Design of Biorefineries	RaG	6-2012	(12-2014)	KAIST, Korea
Shayane Maghalhaes	Study of the enzymatic transesterfication reaction of palm oil and the phase equilibria modeling of biodiesel related mixtures	RaG (Prof F. Pellegrini Pessoa)	3-2013	8-2013	Govenrment of Brazil

MSc-project Students	Project Title	Supervisor	Start	End	Funding
Fabrício Rodrigues	Advances in Process Systems Engineering	RaG/DKB	2-2012	1-2013	Federal University of Uberlândia, Brazil
Kim Braad Carlsen	Stability of Benzon Boilers at Low Load	JA/JKH	8-2012	3-2013	DTU
Amata Anantpinijwatna	Synthesis and design of water and wastewater network for optimal water conservation	RaG/GSI	2-2013	6-2013	Government of Thailand
Rage Mohamed Hersi	Process Intensification Case Studies	RaG	2-2013	6-2013	DTU
Seyed Soheil Mansouri	A Phenomena based Process Intensification – A case study	RaG/JKH	2-2013	6-2013	DTU
Emmanouil Papadakis	Modeling of unsaturated fatty acid oxidation with H2O2	GSI/RaG	2-2013	6-2013	DTU
Muhammad Imran Bin Ismail	Sustainable Biodiesel Process Design from Various Palm Oil Sources	RaG/GSI	2-2013	6-2013	DTU
Ignacio Montero Castro	Feasibility of applying L1-adaptive control and Self-optimizing control for bi	GSI	9-2012	5-2013	DTU
Carina da Costa Lira Gargalo	Sustainable Process Design	RaG	3-2013	8-2013	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	NOY; AMH; LACU; MICU; *Sawitree*		*B D Christian*; Q Chen
B: Product & Process Modelling	**RaG**; GSI; JA; JKH	MMI	ThBis;AMH; NOY; AQ; AKV*;* KreTM*;JAPR;* HBoz; MFad; PChe; *Riccardo B;Andreas Å*	E Papadakis	*L Simasatitkul; M Zaman;K Meyer;M R. Jannerup*
C: Synthesis, Design & Analysis	**GSI**; RaG	*AQ*; NAS	AZM; NOY; IGM; KreTM*;* MICU; DKBabi; HBoz; PChe; *Seyed SM; Amata A; ZBHA*	S S Mansour; A Anantpinijwatna; M I Bin Ismail; R M Hersi; CL Gargalo	*L Simasatitkul*; Q Chen, *B D Christian; K Meyer*
D: Control, Operation & Monitoring	**JKH**; GSI; RaG; (KHC)	MMI	ThBis; KreTM; JAPR;Molle; AKV; *Riccardo B;Andreas Å*	I Grossman, K B Carlsen	*M Zaman*
E: Process & Tools Integration	**GSI**; RaG; JKH	*AQ*	AMH; KreTM; IGM; AKV; KRNH;DKBabi;HBoz; MFadPChe; *Amata A; Seyed SM; ZBHA, Carina,Anjan*	A Anantpinijwatna; CL Gargalo	*M Rizwan*
F: Databases & Numerical Methods	**JA**; RaG		AMH; IGM; MICU; LACU; PChe; *Anjan*	CL Gargalo	*B D Christian*; Q Chen
Currently active	**4**	**3**	**19**	**8**	**6**

1: Research area coordinators are indicated in bold; 2: 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	**CAPEC coworkers& research activities**				
	Faculty[1]	**Post-Docs[2]**	**PhD-students[2]**	**MSc-students[3]**	**Others[4]**
1: Micro reactors	KVG; JW; ULKR		Vijay, Søren, Rolf, Inês, Hilde, Andrijana, Alexandar		
2: Continuous processes	KVG; JW; ULKR	Mathias	Aleksandar; Jason, Vijay		
3: Biocatalytic processes	KVG; JW; ULKR	Mathias	Vijay, Jason, Søren, Rolf, Inês, Marie, Hema, Watson, Kresimir, Rui		
4: Process intensification & intensified unit operations	KVG;JW; ULKR	Mathias	Vijay, Jason, Hilde, Inês		
5: PAT	KVG; JW; ULKR	Rita	Aleksandar		
6: Scale translation	KVG; JW; ULKR	Mathias	Anders		
7: Fermentation	KVG; JW; ULKR	Xavier	Anders, Andrijana, Vijay, Laura		
Currently active (at the annual meeting)	**3**	**3**	**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

Rita Lencastre Fernandes (RLF)

PROCESS
Supervisors: KVG
Start: 3-2013; End: 3-2014

Online sensor model monitoring and maintenance

The amount of data collected during bioprocess manufacturing has increased significantly in the last decades, and will continue increasing in the near future, as more, and more advanced process analytical technology (PAT) sensors (in terms of high-throughput and/or complexity in signal processing) are implemented for online or at-line bioprocess monitoring. Once, for example, NIR sensors are implemented in production lines, the performance of these online sensors, which rely on chemometric models, needs to be routinely assessed. Such assessment is based on comparing the sensor model predictions to laboratory estimations (using more accurate analytical methods) of the properties of interest such as product concentration and/or activity. This project, conducted as part of the BIOPRO initiative, aims at developing modular software tools for assisting PAT specialists in the maintenance of online sensor models: for example, (i) aggregation and aligning data from various sources and formats, (ii) execution of data quality checks and (iii) visualization model performance metrics and results for various for model recalibration scenarios.

Collaborators: Novozymes; DONG Energy; CP Kelco
Supervisor: Krist V. Gernaey

Miguel Mauricio Iglesias (MMI)

PROCESS/CAPEC
Supervisors: KVG/JKH
Start: 1-2013; End: 12-2015

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 (e.g. accumulation at a certain section of the distillation column).
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
Start:-05-2013; End: 04-2015

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 (WWTP) are facing nowadays. These new focus areas/challenges include nutrient recycling & recovery, micropollutant & eco-toxicity removal and energy recovery & greenhouse gases minimization. Based on such models, the project will furthermore aim at finding new ways to operate WWTP facilities in order to live up to the increasingly strict legal demands on treatment performance efficiency, 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, comprising a pre-defined plant layout, simulation models, influent loads, test procedures and evaluation criteria.

Collaborators: Lund University; University of Queensland

Mathias Nordblad (MAN)

PROCESS
Supervisors: JW
Start: 01-12-2008; End: 31-11-2012

Process design and evaluation for enzymatic biodiesel production

Biodiesel is one of the more established renewable fuel alternatives. It is traditionally produced using alkaline catalysis, which comes with certain limitations.
The use of enzymatic catalysis promises several advantages over traditional production method, including higher yields, compatibility with a wider range of oil feedstocks and a safer process. Additionally, the mild reaction conditions also reduce the need for product purification and increase the value of the by-product glycerol. However, the process requires development and optimization to meet criteria for performance and operating costs.
The focus of this project is the reaction and process design for enzymatic biodiesel production, based on evaluation of the performance of individual unit operations and overall process economics. The project is part of, and supported by, a larger collaboration looking into catalyst and reactor performance in enzyme-catalyzed biodiesel reactions, as well as system thermodynamics and sustainability issues.

Collaborators: Emmelev; Novozymes; Aarhus University; DTU Management

Noor Asma Fazli Bin Abdul Samad(NAS)  **CAPEC** Supervisor: RaG Start: 01-10-2012;End: 31-07-2013	***The Rational Selection of Polymers for Pharmaceutical Formulation Design*** In this work, model-based approaches are proposed to predict the miscibility and solubility of the API in binary API-polymer system and ternary API-polymer-solvent system using UNIFAC-FV and Flory Huggins. For the miscibility, the Gibbs free energy of mixing is estimated using both approaches to predict the compatibility and phase stability of the binary or ternary systems. Meanwhile the activity coefficient needed to estimate the solubility of a drug in the binary or ternary systems is calculated using UNIFAC-FV and Flory Huggins. The application of UNIFAC-FV and Flory-Huggins approaches has been tested through various examples of API in binary and ternary systems involving polymer for miscibility/solubility predictions. Research area: A,B

3.4 PhD-Research Project Overview

Deenesh K. Babi (DKBabi)  **CAPEC-PROCESS**	***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. Supervisors: RaG, JW Start: 1/8-2012; End: 30-7-2015 *Research areas: B, C, E*
Vijaya Krishna Bodla (ViKB)  **PROCESS**	***Integrated microfactories for enzyme production*** This project aims to demonstrate that fermentation and biocatalysis can be integrated into a novel leaner and greener process. The hypothesis is to construct and operate integrated microscale reactors using transaminase model system (adapted to specific microorganism and the biocatalytic reaction) in an intensified and more efficient process also for scaling-up.It is the intention to use an integrated microfactory to quickly and effectively screen for different process conditions. The proposed microfactory has a number of features that are advantageous for large-scale production with respect to improved economy of the proposed process: (1) the method for preparing the catalyst is considerably cheaper as no intermediary purification steps are needed; (2) the system process intensity is inherently enhanced through the continuous operation; (3) large hydrophobic substrates would be easily accessible since the cell membranes are lysed. Supervisors: KVG,ULKR,JW Start: 01-03-2011; End: 28-02-2014 *Research area: Microreactors; Biocatalysis*

Thomas Bisgaard (THBIS)

CAPEC

Operation and design of diabatic separation processes

Multi-stage distillation is the most widely used industrial technique for continuously separating liquid mixtures. At the same time it is an energy intensive operation, so the technology still receives attention due to increased focus on environmental issues and resource management. Studies reveal that conventional distillation columns operate at Second-Law efficiencies in the range of 5-20%. Various alternative distillation column configurations with higher Second-Law efficiencies have been suggested. A promising group of alternative configurations are the diabatic distillation columns which will be subject of this PhD project. Extensive efforts have been conducted to develop the diabatic distillation technology since the late 70's. Despite demonstrations of large energy savings of e.g. the HIDiC compared to the CDiC and manageable operability, it has not yet been accepted by the industry. This could be due to lack of mature methods for designing these more complex configurations. Furthermore operation is more complex as a result of the high degree of process integration. The main goal of this project is to reap the benefits of diabatization of distillation column, and to identify and hopefully reduce its bottle necks in the commercialization.

Supervisors: JKH, JA, KIPI, NVS
Research Areas: B, C, F
Start: 1-09 2012; End: 31-08-2015

Hande Bozkurt (HBOZ)

CAPEC-PROCESS

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.

Supervisors: GSI, KVG
Start: 16-12-2011; End: 16-01-2015
Research area: B,C, E

Peam Cheali (PCHE)

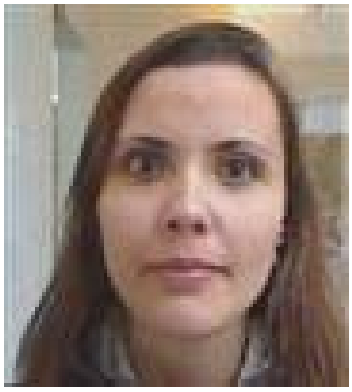
CAPEC-PROCESS

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.

Supervisors: GSI, KVG
Start: 01-05-2012; End: 31-05-2015
Research area: B, C, E

Larissa P Cunico (LACU)



CAPEC

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.

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

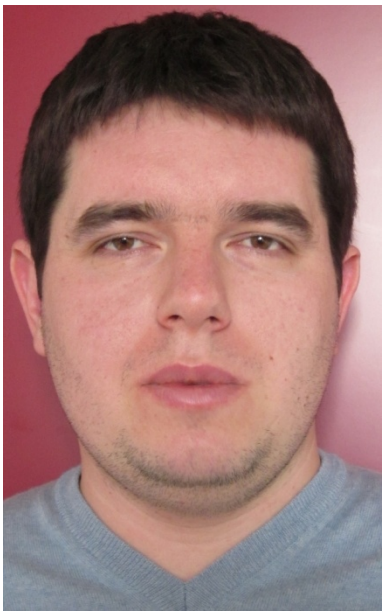
Marina Fedorova (MFAD)  **CAPEC**	***Systematic methods and tools for computer aided modelling*** Models play an important role of increasing importance in design and analysis of chemicals/bio-chemicals based products and the processes that manufacture them because of the increasing use of computer-aided 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. Supervisors: RaG, GSI Start: 1-4-2012; End: 31-3-2015 *Research areas: B, E, F*
Zainatul Bahiyah Binti Handani (ZBHA)  **CAPEC**	***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. Supervisors: RaG, GSI Start: 1-6-2013; End: 31-5-2016 Research area: B, C, E

Søren Heintz (SHEIN)  **PROCESS**	***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). Supervisors: KVG, JW, ULKR, PT BIOINTENSE EU-funded 7th Framework project
Amol S Hukkerikar (AMH)  **CAPEC**	***Model based integrated process-product design - retrofitting and optimisation*** The main objective of this project is to develop a systematic framework for model based design and optimisations of the principal unit operations involved in edible oil/bio-fuel industry and apply the developed methodology for improvement in the performance of existing installations for edible oil/bio-fuel processes. Although the oleo-chemical industry is mature and based on well established processes, the complex systems that lipids compounds form, and the lack of accurate unit operation models have limited a wide application of computer aided methods and tools for process synthesis, modeling and simulation within this industry. In consequence, the first part of this project will be the development of unit operations model library consisting of a collection of new and adopted models that are not available in existing process simulation tools. The second part of the work will focus on application of developed models for optimisation of existing processes with respect to performance indicators such as minimum operational cost, product yield improvement and sustainability index. Supervisors: RaG, GSI, Bent Sarup (Alfa Laval). Started: 01-07-2010; Finish: 30-06-2013 *Research area: A, B, C, E*

Sawitree Kalakul (SKALA)  **CAPEC**	***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. Supervisors: RaG, Bet Sarup, Georgios Kontogeorgis Start: 1-6-2013; End: 31-5-2016 *Research areas: A, B, C*
Hilde Larsson (HILA)  **PROCESS**	***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. Supervisors: ULKR, KVG, Anne Ladegaard Skov

Michele Mattei (MICU)  **CAPEC**	***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. Supervisors: RaG, G. Kontogeorgis (AT-CERE) Start: 1/8-2012; End: 30-7-2015 *Research areas: A, C, F*
Kresten T. Meisler (KRETM)  **CAPEC-PROCESS**	***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. Supervisors: RaG, KVG, NvS Start: 01-03-2011; End: 28-02-2014 *Research area: B, C, D*

Aleksandar Mitic (ASMI)



PROCESS

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.

Supervisors: KVG, Kim Dam-Johansen (CHEC)
Start: 15-11-2010; End: 14-11-2013
Research area: continuous pharmaceutical production, PAT, microreactor technology

Igor Mitrofanov (IGM)

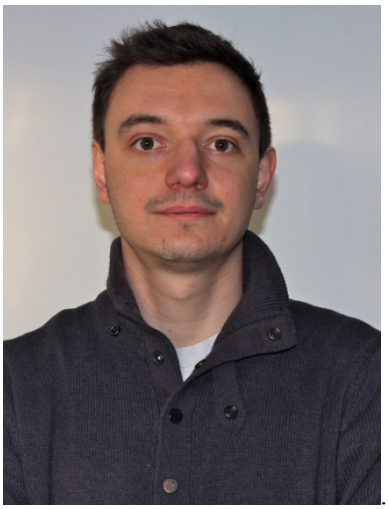
CAPEC

A methodology for systematic design and selection of green solvents for increased yield in organic reactions

Methodology for selection and design of single organic reactions has previously been developed at CAPEC (Gani et al, Computers and Chemical Engineering, 2005, 2008). This methodology is based on a rule-based algorithm. However, the methodology is applicable only to organic chemicals that are inert within the reaction system. The next step is extending the application range of current methodology to multi-stage reactions (because, for example, pharmaceutical reactions are normally multi-step), more complex reaction systems, known solvent substitution problems as well as reaction promotion.

Supervisors: RaG; GSI, JA
Start: 01-11-2010; End: 4-10-2013 (stopped)
Research area: C, E, F

Ane H Mollerup (MOLLE)  **CAPEC**	***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). Supervisors: GSI, Peter S Mikkelsen, Dines Thornberg Start: 1-8- 2011; End: 1-8-2014 *Research area: B, D*
Anders Nørregaard (ANDNO)  **PROCESS**	***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. Supervisors: KVG, JW, Sturat M. Stocks, Brian Madsen, Frans van den Berg

Jason Price (JAPR)  **CAPEC-PROCESS**	***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. Supervisors: JW, JKH, MAN Start: 01-09-2011; End: 01-10-2014 *Research area: B, D*
Alberto Quaglia (AQ)  **CAPEC**	***Incremental refinement of process design*** Process Simulation is not common in the food and biofuels industries, mainly due to the complexity of thermodynamics and transport properties of the species involved. This project aims to introduce a paradigm shift in product-process design through the application of CAPE/PSE tools in these industries. The research will focus on the use of validated models in the early stages of product-process design in order to eliminate redundant alternative process routes. The objective will be to identify the most promising process route so that the more time consuming and costly steps (computational as well as experimental) can be reduced. To achieve this objective, a systematic framework for Computer-Aided Flowsheet Synthesis and Design (CAFD) will be developed and evaluated in collaboration with Alfa Laval. A particular emphasize will be given to deal with uncertainties in data and models. Supervisors: GSI, RaG, Bent Sarup (Alfa Laval) Start: 01-06-2010; End: 31-05-2013 *Research area: B, C, E*

Rolf Hoffmeyer Ringborg (ROLRI)  **PROCESS**	**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. Supervisors: JW, KVG, ULKR BIOINTENSE EU-funded 7th Framework project
Ines Periera Rosinha (INROS)  **PROCESS**	***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. Supervisors: ULKR, JW, KVG, Anders Daugaard

Laura Snip (LASN)

PROCESS

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

The project has focus on wastewater treatment plant (WWTP) models, and aims at studying and implementing mathematical models concerning both the prediction of greenhouse gas emissions from the WWPT and the fate of micropollutants in the WWTP. Models will be obtained from the literature, and will be implemented in the Benchmark Simulation Model no. 2 (BSM2). BSM2 is a general plant wide model of a WWTP that was developed in order to compare different control strategies. The model includes a plant layout, a simulation model, influent loads, test procedures and evaluation criteria, which will ensure outcomes of different control strategies that will be comparable. Once the models extension is accomplished, different scenarios will be compared according to newly developed evaluation tools. These evaluation tools should include criteria concerning greenhouse gas 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.

Supervisors: KVG, ULKR, XFA, Ulf Jeppsson, Benedek Plosz
Start: 1/5-2012; End: 30-4-2015
Research areas: Fermentation

Anna Katrine Vangsgaard (AKV)

CAPEC-PROCESS

Validation of structured model for autotrophic nitrogen removal in high strength wastewater

Autotrophic nitrogen removal is a relatively new and emerging technology for treatment of sidestream wastewaters with high nitrogen concentrations, such as sludge digestion liquor or landfill leachate. It is therefore of great importance that a better understanding of the process dynamics is established. In this project, a model to be used for design of experiments will be developed according to a structured modeling framework. The aim of this project is to develop a detailed metabolic model for the selected bacterial groups, performing autotrophic nitrogen conversion, and integrate that into complete ecosystems models, which describe how the major microbial groups interact. This insight will be used to design experiments in which relevant operational conditions will be identified and tested. The relevant conditions are under which the nitrogen removal process is optimized through the development of selection principles, for a targeted removal or enhancement of specific microbial groups. The final objective is to obtain a validated model which can be used for process prediction and thus determination of optimal operational conditions.

Supervisors: GSI, KVG, Barth F. Smets
Started: 01-09-2010; Finish: 31-08-2013
Research area: B, E

Nor Alafiza Yunus (NOY)  **CAPEC-PROCESS**	***Tailor-made design of chemical products: Bio-fuel and other blended products*** This study proposes a methodology for tailor-made design of chemical products more specifically bio-fuels and other blended products. This project emphasize on product blends because most of the chemical based products are mixed of several chemicals. A single chemical is not always able to meet all the product specifications. Therefore, a mixture/blend of chemicals is likely to improve and enhance the product qualities. Identifying mix; ture of appropriately identified compounds that satisfied product attributes is the main goal of this study. In order to achieve the objectives, four key tasks are needed. Firstly, the general chemical blending problem is formulated. Then, the property models are identified to estimate the pure and mixture properties. The unavailable property models are being developed by using experimental data and appropriate modeling tools. Next, the chemical mixture/blend algorithm is developed in order to find the best mixture/blend using suitable solution strategy. Finally, the developed mixture/blend algorithm is applied to case studies and validated with experimental data. Supervisors: RAG, JW, KVG Start: 01-06-2010; End: 01-05-2013 *Research area: A, B, C*
Rui Xue (RXUE)  **PROCESS**	**Reactor and process design for multi-step biocatalysis** Biocatalysis has become increasingly attractive for the development of more efficient and cleaner chemical synthetic processes. Higher selectivity and specificity, as well as the use of mild reaction conditions in general gives an excellent ‘green’ profile to reactions catalyzed by enzymes. In this project, the synthesis of sialic acid derivatives will be taken as an example for the design of an enzyme cascade. Laboratory scale-down tests will be carried out to characterize the enzymatic systems. Engineering tools for the selection of synthetic routes, reactors and processes will be developed for the reactions which involve multi-step biocatalysis. Supervisor: JW Start: 12-2010; End: 11-2013

3.4 External PhD-students (projects)

Shayane Magalhaes  **UFRJ (Brazil) -CAPEC**	***Study of the enzymatic transesterification reaction of palm oil and the phase equilibria modelling of biodiesel related mixtures*** In this project, the focus is given toward biodiesel production from palm oil since its production has a high energy efficiency factor and a high yield per hectare. In addition to methanol, bioethanol produced from sugarcane will also be considered since it is nontoxic; the carbon of the obtained biodiesel is 100% of renewable sources, and is largely available in Brazil. Enzymatic catalyst, such as lipases will be considered for the transesterification of the palm oil to biodiesel. In order to understand and control the variables that affect the process, the phase behavior involved in the reaction and purification steps will be studied in detail. Therefore, the main objective of this project is to study the biodiesel production process via enzymatic ethanolysis of palm oil. Thus, kinetics, vapor-liquid and liquid-liquid equilibrium (VLE, LLE) data have been obtained experimentally. Based on these, the mathematical modeling of reactors and separation processes will be made. Furthermore, the economical evaluation to assess the costs of biodiesel production via enzymatic route will also be studied. Collaboration with Universidad Federal Rio de Jeneiro (UFRJ), Brazil (Prof F Pellegrini Pessoa); RaG March-August, 2013 *Research areas: A*
Muhammad Rizwan  **KAIST-CAPEC**	***Superstructure optimization of biodiesel production from microalgal biomass*** In this study, a mixed integer nonlinear programming (MINLP) model for superstructure based optimization of biodiesel production from microalgal biomass is beoing developed. The superstructure includes a number of major processing steps for the production of biodiesel from microalgal biomass, such as harvesting of microalgal biomass, pretreatments including drying and cell disruption of harvested biomass, lipid extraction, transesterification, and post-transesterfication purification. The developed model is used to find the optimal processing pathway among the large number of potential pathways that exist for the production of biodiesel from microalgae. The proposed methodology is being tested by implementing it on a specific case study. The MINLP model is implemented and solved in GAMS using a database built in Excel. Collaboration with KAIST, Korea (Prof Jay H Lee) *Research areas: B, E*

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 nothave 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 16.0

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 16.0, 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**algorisare 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

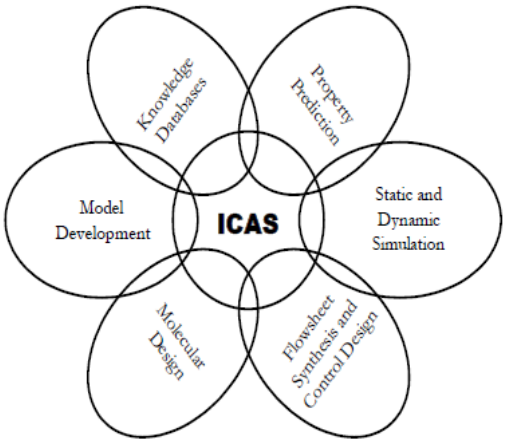


Figure 4.1:The idea of integration within **ICAS**

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).

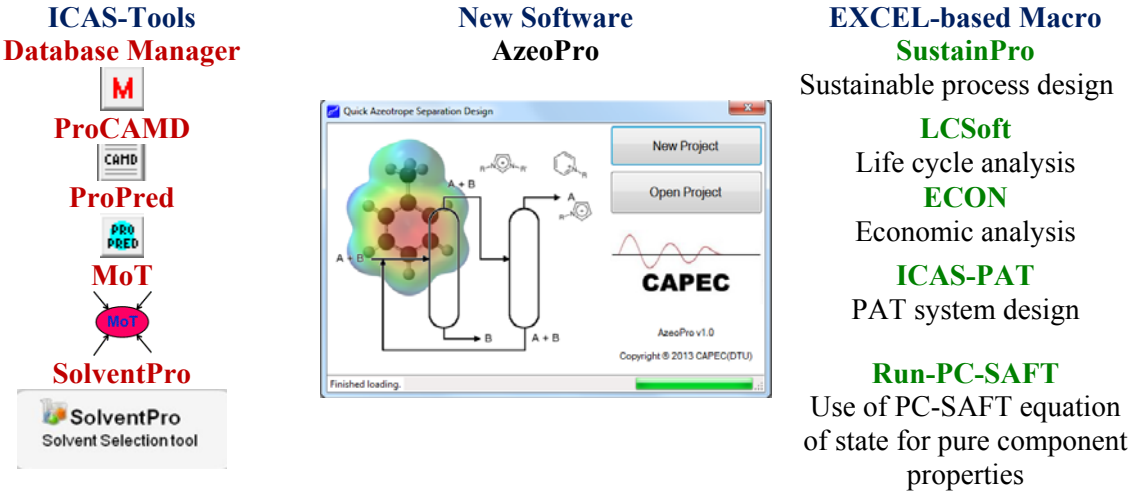


Figure 4.2: Highlight of new features in ICAS 16.0

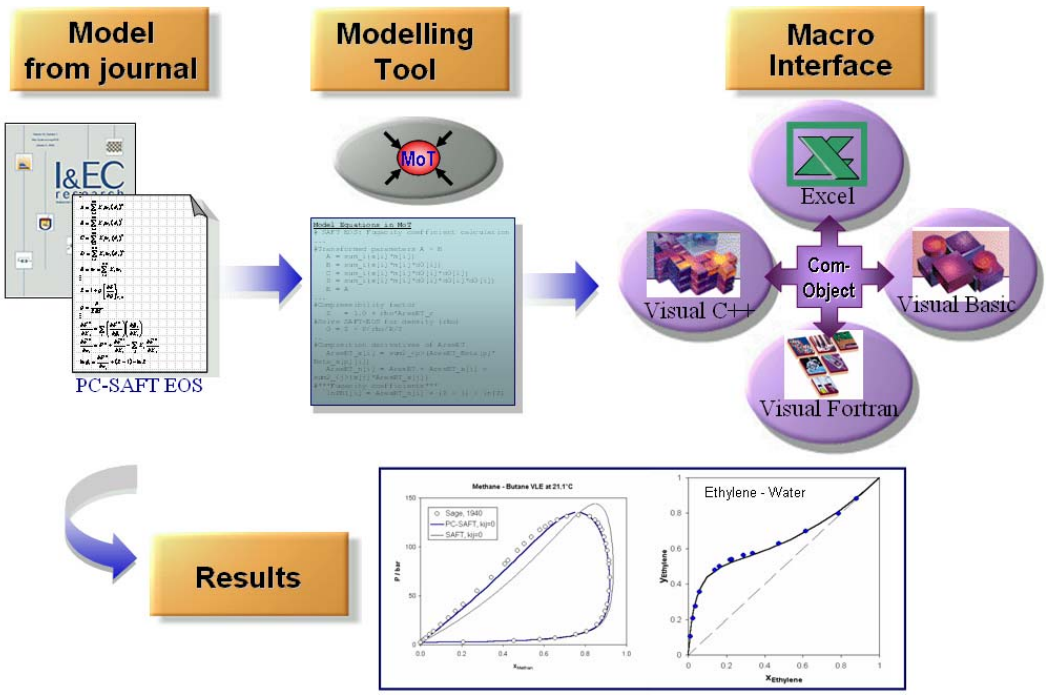


Figure 4.3: COM-object generation through MoT and use in external software

In ICAS 16.0, MoT has new features (see the MoT new features document); ProCamdand SolventPro have had bug-fixes; a new solvents database has been added to the CAPECDB (EXCEL version);andSustainPro and theLCSoft have new versions.

In ICAS 16.0, 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).

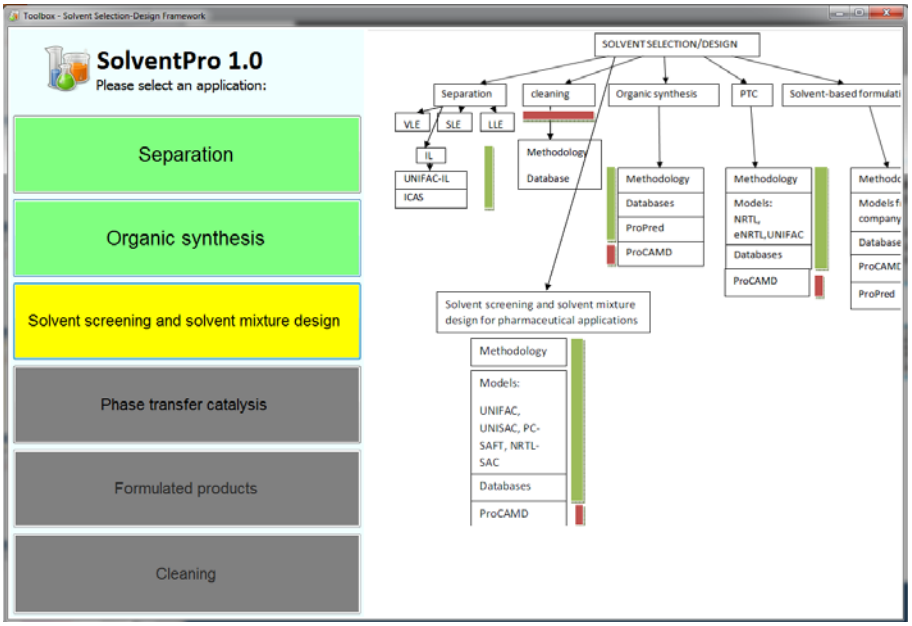


Figure 4.4: New feature of SolventPro (highlighted in yellow)

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.

4.4EXCEL-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.

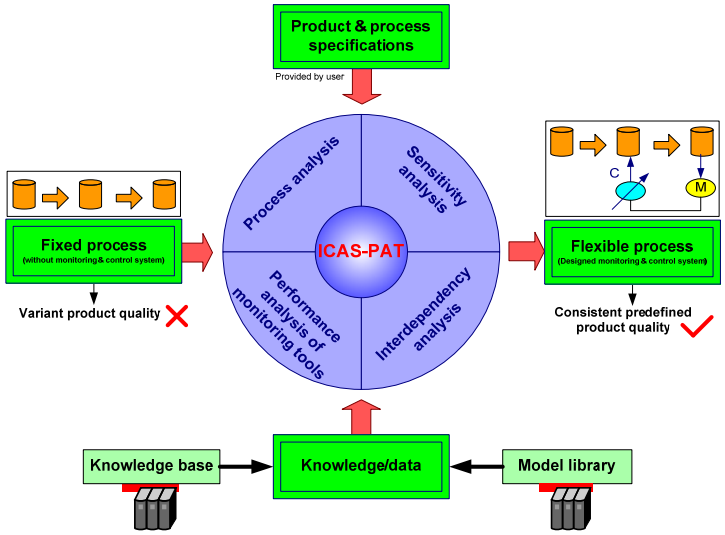


Figure 4.5a: Overview of the main features of ICAS-PAT.

SustainPro

SustainPro is an EXCELbased software, which provides options for retrofit analysis and performance analysis of a given process. A new version is now available with more automated

stepsand a number of worked out examples. The objective is to perform sustainable process design through SustainPro (see also PEC12-55).

As highlighted in Fig 4.5b, 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. As it can be seen from Fig 4.5b, the two options can be combined, which means that they complement each other. After applying the retrofit analysis, the performance analysis is performed and compared with the base case design.

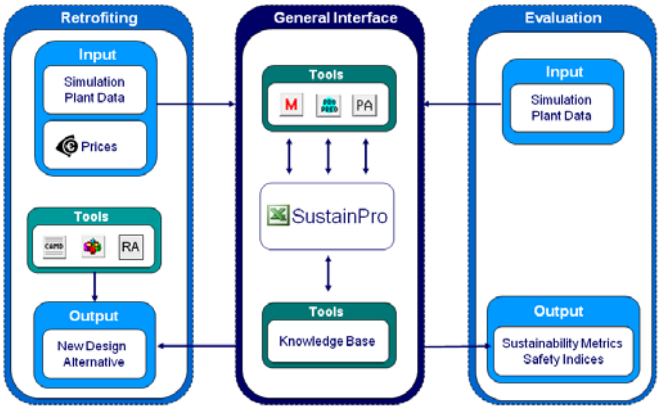


Figure 4.5b: Overview of the main features of SustainPro

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 4.4cgives 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.

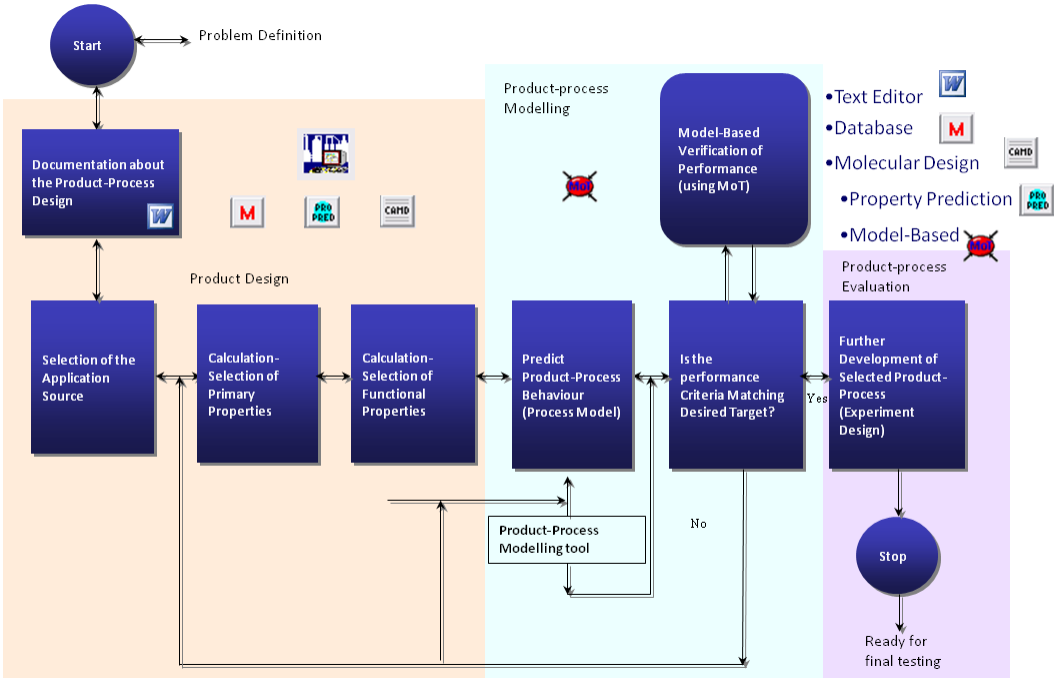


Figure 4.4c: The virtual product-process design lab

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).

A new option has been made available in Propred 4.4to run PC-SAFT for the calculation of the temperature dependent properties of pure components.

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 doinga list by property or a property search (duplicates are removed).

5. Research highlights (2012-2013)

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*Noor Asam Fazli Bin Abdul Samad, 2012, "Control of Process Operations andMonitoring of Product Qualities through Generic Model-based Framework inCrystallization Processes", PhD-thesis(PEC12-40) – CAPEC-PROCESS*

A generic and systematic model-based framework for the design of a process monitoring and control system to achieve the desired crystal size distribution (CSD) and crystalshape for a wide range of crystallization processes has been developed. This frameworkcombines a generic multi-dimensional modelling framework, tools for design of set pointprofiles, for design of PAT (Process Analytical Technology) systems as well as option toperform the uncertainty and sensitivity analysis of the PAT system design. Through thisframework, it is possible for a wide range of crystallization processes to generate thenecessary problem-system specific model, the necessary set point using the extendedanalytical CSD estimator and the response surface method (RSM) and a PAT systemdesign including implementation of monitoring tools and control strategies in order toproduce a desired product with its corresponding target properties. In addition the impactand influence of input uncertainties on the predicted PAT system performance can bequantified, i.e. the risk of not achieving the target specifications of the crystal product canalso be investigated. The application of the systematic model-based framework is dividedinto three sections: a) the application of the generic multi-dimensional modeling framework are highlighted: i) the capability to develop and further extend a batch coolingcrystallization model is illustrated through a paracetamol case study, supplemented by asucrose crystallization example to demonstrate how the framework supports smoothswitching between chemical systems with a minimum modelling effort; ii) a potassiumdihydrogen phosphate (KDP) case study is used to demonstrate how the modelcomplexity can be increased, that is, by switching from a one-dimensional to a twodimensionaldescription; b) the systematic framework is used in a case study to design a monitoring and control (PAT) system for a potassium dichromate and KDPcrystallization processes to achieve the desired target CSD respectively; and c) Based onthe PAT system design in b), the application of uncertainty and sensitivity analysis isthen highlighted for the potassium dichromate and KDP crystallization process both inopen-loop and closed-loop operation. In the case study, the impact of input uncertaintiesrelated to parameters of the nucleation and the crystal growth model on the predictedsystem performance has been investigated for a one- and two-dimensional CSD and itshown the PAT system design is reliable and robust under considered uncertainties.

5.1.2*Azizul Azri Bin Mustaffa, 2013,* "Development and Analysis of Group Contribution^{Plus} Models for Property Prediction of Organic Chemical Systems*", PhD-thesis (PEC12-60)- CAPEC*

Prediction of properties is important in chemical process-product design. Reliable property models are needed for increasingly complex and wider range of chemicals. Group-contribution methods provide useful tool but there is a need to validate them and improve their accuracy when c omplex chemicals are present in the mixtures. In accordance with that, a combined group-contribution and atom connectivity approach that is able to extend the application range of property models has been developed for mixture properties. This so-called Group-ContributionPlus (GCPlus) approach is a hybrid model which combines group contribution and molecular descriptor theories (such as connectivity indices – CI). Connectivity indices are formalisms defined via graph theoretical concepts intended to describe the topological characteristics of molecular structures. The main idea is the use of connectivity indices to describe the molecular fragmentation that relates properties which is the molecular interactions with the molecular structures. One well known and established group-contribution method is the UNIFAC model, used to predict liquid phase activity coefficients

for mixtures. The needed values of the group interaction parameters (GIPs) are obtained by fitting phase equilibrium data. There are, however many gaps in the UNIFAC parameter table due to lack of data. Alternative to performing measurements, which may not be feasible, values of the missing GIPs, can be predicted through the GCPlus approach. The predicted values for the GIPs are then used in the UNIFAC model to calculate activity coefficients. This approach can increase the application range of any "host" UNIFAC model by providing a reliable predictive model towards fast and efficient product development. This PhD project is focused on the analysis and further development of the GCPlus approach for predicting mixture properties to be called the UNIFAC-CI model. The contributions of this work include an analysis of the developed Original UNIFAC-CI model in order to investigate why the model does not perform as well as the reference UNIFAC model for some systems while performing surprisingly better than the reference model for other systems. In this analysis, it is found that by introducing more structural information to the CHO group through the valence connectivity index (CI), the correlation error involving alkanes-aldehydes system can be reduced. Furthermore, as a continuation of the analysis done for systems involving C, H and O atoms, the Original UNIFAC-CI (VLE) model has been further reused and significantly expanded by including nitrogenated, chlorinated and sulfurated systems and the involved atom interaction parameters (AIPs) have been regressed. In addition to that, another set of parameters have been generated for the Original UNIFAC-CI (VLE) model using a quality assessment algorithm, QVLE (combination of 4 VLE consistency tests) as a weighting factor for each VLE dataset in the objective function for regression of AIPs. The quality factors are useful in identifying anomalous systems which can be problematic in the parameter estimation and can produce parameters which are not accurately representing the systems used for the regression. The thesis has also determined parameters for the Original UNIFAC-CI (VLE/SLE) model through regression against both VLE and SLE experimental data. The prediction accuracy of SLE systems using the regressed parameters has been slightly increased. Also, the Modified (Dortmund) UNIFAC-CI has been further developed by including chlorinated and sulfurated VLE systems, and, the developed Original UNIFAC-CI (VLE/SLE) model has been highlighted in selected case studies involving the design of a working solution for hydrogen peroxide production and solubility investigation of pharmaceutical systems where new group have been created and their interaction parameters are predicted/fine tuned generating a master parameter table specifically for those case studies. Also, the applicability of the Original UNIFACCI model is shown for predicting phase equilibria of lipid systems, filling missing GIPs and improving prediction of azeotropic mixture.

5.1.3 Rita Lencastre Fernandes, 2013, "Modeling Approaches for DescribingMicrobial Population Heterogeneity", PhD-thesis –PROCESS

Although microbial populations are typically described by averaged properties,individual cells present a certain degree of variability. Indeed, initially clonal microbial populations develop into heterogeneous populations, even when growing in a homogeneous environment.

A heterogeneous microbial population consists of cells in different states, and it implies a heterogeneous distribution of activities (e.g. respiration, product yield), including different responses to extracellular stimuli. The existence of a heterogeneous cell population may explain the lower productivities obtained for cultivations in large-scale reactors, where substrate and oxygen gradients are observed, in comparison to cultivations in well-mixed bench scale reactors.

Population balance models (PBM) have been used in a broad range of applications (e.g. crystallization, granulation, flocculation, polymerization processes) to predict distributions of certain population properties including particle size, mass or volume, and molecular weight. Similarly, PBM allow for a mathematical description of distributed cell properties within microbial populations. Cell total protein content distributions (a measure of cell mass) have been observed to provide a dynamic picture of the interplay between the cells and their surrounding extracellular environment.

The work here presented aimed at developing a model framework based on PBM as a tool to further understand the development of heterogeneous microbial populations subjected to varying environmental conditions. Three cases are presented and discussed in this thesis. Common to all is the use of *S. cerevisiae*as model organism, and the use of cell size and cell cycle position as single-cell descriptors.

The first case focuses on the experimental and mathematical description of a yeast population dynamics, in response to the substrate consumption observed during batch cultivation. Cell size and cell cycle position distributions were used to describe the cell population. A two-stage PBM was developed and coupled to an unstructured model describing the extracellular environment. The good agreement between the proposed multi-scale model and experimental data (both the overall physiology and cell size and cell cycle distributions) indicates that a mechanistic model framework is a suitable tool for describing the microbial population dynamics in a bioreactor.

The second case provides an extension of the proposed model framework (PBM coupled to an unstructured model) to a continuous cultivation. A compartment model approach was applied for addressing situations where two zones (compartments) are formed due to non-ideal mixing in the bioreactor. In particular, this approach was used in order to assess the impact of the degree of compartmentalization (i.e. deviation from the ideal mixing case) on the population dynamics and overall system performance under various operation conditions (substrate feed concentration and dilution rate). It was possible to conclude that the deviation from ideal mixing may have a significant effect on the observed system dynamics. Moreover, oscillatory pseudo-steady states may be observed for particular combinations of operating conditions and degree of compartmentalization.

In the third study attention was paid to the integration of the proposed model framework in a computational (CFD) fluid dynamic model. The anaerobic growth of a budding yeast population in a continuously run microbioreactor was used as example. The proposed integrated model describes the fluid flow, the local cell size and cell cycle position distributions, as well as the local concentrations of glucose, ethanol and biomass throughout the reactor. This work has proven that the integration of CFD and population balance models, for describing the growth of a microbial population in a spatially heterogeneous reactor, is feasible, and that valuable insight on the interplay between flow and the dynamics of a budding yeast population (e.g. formation of substrate gradients and non-growth zones) is gained. *In silico*simulation tools, as the one proposed, may be used for hypothesis generation and testing, and when coupled to an experimental set-up may be usedfor process and reactor design optimization.

5.1.4*Joana Lima-Ramos****,*** *2013, "*A methodology for development of biocatalytic processes*", PhD-thesis- PROCESS*

The potential advantages displayed by biocatalytic processes for organic synthesis (such as exquisite selectivity under mild operating conditions), have prompted the increasing number of processes running on a commercial scale. However, biocatalysis is still a fairly underutilised technology. As a relatively new technology biocatalytic processes often do not immediately fulfil the required process metrics that are key for an economically and/or environmentally competitive process at an industrial scale (high concentration, high reaction yield, high space-time-yield and high biocatalyst yield). However, these process metrics can often be attained by improvements in the reaction chemistry, the biocatalyst,and/or by process engineering, which often requires a complex process development strategy. Interestingly this complexity, which arises from the need for integration of biological and process technologies, is also the source of the greatest opportunities. Indeed, recombinant DNA technology offers a superb complement to process technologies. Potentially this is one of the biggest advantages of biocatalysis when compared with conventional chemical catalysis, where all the reaction boundaries are fixed by the physical and thermodynamic properties of the reaction compounds. Therefore, the main avenue that still remains

to be explored by process engineers is how to promote process development ina systematic way rather than on a case-by-case basis, as is frequently the case today.

One of the main challenges in process development is selecting between different process alternatives. The development effort for a novel process is considerable and thus, an increasing number of conceptual process design methods are now applied in chemical industries. Since the natural environment of the biocatalyst is often very different from the operating conditions suitable for a viable process (high substrate and product concentrations, unnatural substrates, presence of organic solvents, etc.), process development strategies are particularly relevant for biocatalytic processes. However, state-of-the-art methodologies for process development applied to biocatalysis often prove to be unsuccessful. At the early development stage the biocatalysts are usually still under development and many of the reactions have not yet achieved their full potential, many of the process technologies are not yet well described and their relationship with the overall process is not clear.

The work described in this thesis presents a methodological approach for early stage development of biocatalytic processes, understanding and dealing with the reaction, biocatalyst and process constraints. When applied, this methodology has a decisive role in helping to identify many of the process bottlenecks up-front and in a straightforward way, whilst indicating development targets, allowing a better use of resources and shortening development time. The methodology is illustrated through three different case studies: α-caprolactam production by a multi-enzymatic process, chiral amine production using ω-transaminase and finally long-chain chiral aliphatic alcohol production by a bi-enzymatic system. For each case study presented, a different tool is used to guide development and evaluate the process when different levels of underlying process knowledge are available.

The first case study presents a rational approach for defining a development strategy for multi-enzymatic processes. The proposed methodology requires a profound and structured knowledge of the multienzyme systems, integrating chemistry, biological and process engineering. In order to suggest a reduced number of feasible process design options, cofactor and interaction matrices are used, identifying the challenges and addressing them by selecting appropriate process configurations. Based on this information, feasible flowsheets and mass and energy balances are identified. By applying evaluation tools (economic and environmental analysis), the number of options can be much reduced and the current process bottlenecks identified. By applying *a priori* this methodology, the laboratory experts are better able to understand the most favourable operating conditions at full-scale and thus be able to collect information at these relevant conditions.

In the second case study, windows of operation are used to quantify and visualise process performance and feasibility when interactions between process technologies and biocatalyst performance (or reaction) are significant. The methodology constitutes a useful tool that provides easy interpretable results to enable rational design choices of different available process technologies. In the particular case of the asymmetric synthesis of chiral amines, the reaction constraints (thermodynamic equilibrium) must be solved prior to implementation and these fix the hard boundaries of the operating space. Further, improvements in the biocatalyst specific activity are also required for a successful full-scale implementation.

In the third case study a methodology for bottleneck analysis is presented, incorporating process modelling and engineering evaluation tools. The benefit of such models, when integrated with evaluation tools, is that they can be used to predict the process performance and identify bottlenecks, without requiring experimental examination thereby reducing the resources and time for process development. The use of this methodology in the context of reaction engineering is to propose new operating conditions at which the process performance is improved, while identifying the remaining bottlenecks and suggesting further research efforts.

Although the proposed methodology is still in its infancy when compared with other established process development tools and methods, it provides a good overview of the whole reaction system and process. Furthermore, the proposed methodological approach establishes a systematic evaluation of different process options (e.g. flowsheets) and indicates required fundamental data collection and development efforts for further development stage. However, this methodology could be greatly enhanced by the implementation and integration of *in-silico*tools for property and thermodynamic data as well as process mechanistic models to assist in the selection of process technologies.

5.1.5*Naweed Al-Haque**, 2013, "*Integrating porous resins in enzymatic processes*", PhD-thesis (PEC13-35) - PROCESS-CAPEC*

Increasing pressure mandated by different government policies, for developing sustainable chemical processes for the synthesis of optically pure compounds, has resulted in increased considerations of biocatalysis as a viable option by many industries. Biocatalysis, with its exquisite selective properties and potential 'green' attributes, presents it as a sustainable alternative. Today, the role of biocatalysis is most evident in the pharmaceutical industry and is currently extending towards fine and bulk chemical production as well. The use of hydrolytic enzymes (lipases) is well established in several chemical industries, though certain challenges persist in other types of enzymes (transferases and ketoreductases), thus limiting their implementation in industry. Inhibition by substrate and product as well as low aqueous solubility of substrates has constrained the full potential of these enzymes to be harnessed.

To overcome these challenges, different process strategies are required to obtain high yields. A number of different challenges and proposed solutions are discussed in chapter one of this thesis and have also been published as a review. In recent years, integrating porous resins as an auxiliary phase in enzymatic processes, to non-selectively bind the substrate and product as a means to alleviate substrate and product inhibition, has gained considerable recognition. The resins act as a reservoir for the inhibitory substrate and a sink for the inhibitory product and simultaneously attain the required high substrate loading to make the process economically feasible. In this way the potential benefit of the enzyme can be exploited.

Porous resins as opposed to other auxiliary phases, for example organic solvents, are nonbioavailable, biocompatible and offer simpler operational handling (no foaming and emulsification). This strategy has been applied effectively to single substrate – single product systems (oxidation, degradation and hydrolysis). However, this concept has not been extended to other industrially relevant reactions which are two substrate – two product systems.
In this thesis, a methodological framework has been successfully developed to aid in implementing the strategy of integrating porous resin for multi-component systems. In this manner, a generic platform has been established for biocatalytic reactions that require the integration of this strategy. The framework identifies the key information about the reaction and the process using a step-wise protocol with the required tools. It includes the use of kinetic modelling in characterizing the reaction kinetics, a heuristic approach for screening resins and a model based approach for evaluating the process. Greater knowledge about the enzymatic processes with integrated porous resins can therefore be gained and thus the efficiency of process development with respect to time and resources required (reduced number of experiments) could be increased.

Estimating kinetic model parameters for enzymatic reactions is quite complex and frequently leads to identifiability issues. In order to understand the different techniques to estimate the parameters, a number of concepts are discussed in chapter four of this thesis. This knowledge has contributed tothe development of a robust methodology for the estimation of kinetic model parameters for biocatalytic reactions, which has also been published in a peer reviewed journal.

Screening resins for moderately hydrophobic multi-component systems is challenging. Often it is found that the capacity of the resin is inversely related with product selectivity. Therefore a tradeoff has to be made between these parameters which can be crucial from an economic point of view. A low resin capacity points towards the need for higher resin loading, which in turn determines the equilibrium concentration of the substrate in the reactor and the type of reactor that can be used (stirred tank reactor or packed bed reactor). Similarly low product selectivity would result in higher product concentration in the reactor and thus not aid in alleviating inhibition. Further considerations of resin stability and cost also have to be taken into account in the screening procedure. The screening therefore becomes a multi-objective task that has to be solved simultaneously. Such an approach has been applied in the method formulated in this framework.

Process modelling is a very effective tool in evaluating a process. Critical information about the process can be gained by means of simulations, which can further be re-used to tune the reaction or process conditions to harness the full potential of the enzyme. State-of-the-art mathematical techniques for model quality evaluation, such as uncertainty and sensitivity analysis, have been included in this analysis in order to identify the key model parameters for better understanding of the process.

Three case studies were used to illustrate the applicability of the methodology to fulfil different objective requirements. The case studies were selected for not only being industrially relevant but as well as having certain limitations which contributed in developing the tools and strategies to overcome them. The asymmetric synthesis of 1-phenylethylamine using ω-transaminse, the asymmetric synthesis of 1-methyl-3-phenylpropylamine using ω-transaminse and enantioselective synthesis of 2-octanol using alcohol dehydrogenase were selected.

5.2 Publication Record

The last 12-months have seen a big increase for CAPEC in the number of peer-reviewed journal publications. 37+published paper from 2012 to present (plus 30+ “in press” or “submitted”) have been published in major chemical engineering journals (see Appendix 7.3). There have been 11plenary or keynote lectures international conferences and 95+ presentations have been made in important international conferences. 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 16.0 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 (*eg.*, 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 (*eg*., bio-refinery and green chemistry).
- How to develop and provide the necessary models, methods and tools through which the future problems can be addressed (*eg.*,multiscale modelling & integration/intensification)?

CAPEC and PROCESS plans 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 with significantly less time and resources than current practice.
- Product-process design: Use of a multidisciplinary 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

6.3Managing 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).

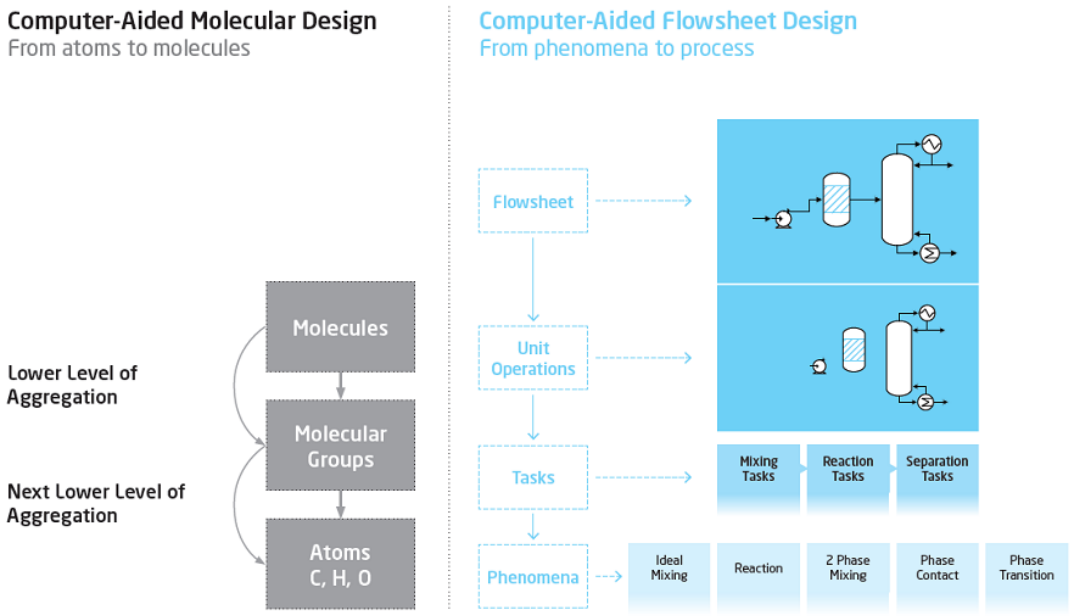


Figure 6.1: Multiscale nature of product-process design problems

Another example of managing the complexity is shown through Fig 6.2, where the complexity of the enterprise wide operations and optimisation problems are represented as a network-of-networksWithin this representation, the enterprise is modelled as a network of processingnetworks, each of them constituted by a network of processing plants, constitutedby a sequence of one or more processes and going into lower scales.

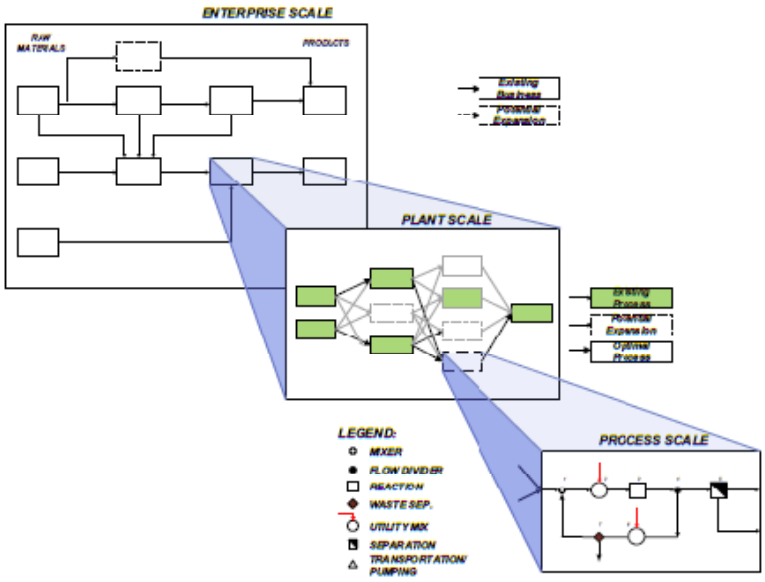


Figure 6.2: Multiscale nature of enterprise wide operations in processing industries

6.4 Some specific plans (CAPEC-PROCESScoworkers) 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 a laboratory in building 227 and also the pilot hall in building 228. The possibility of batch, fed-tach and continuous process operations of biocatalystic reactions at miniature, lab and pilot scale is being developed. Both packed bed and stirred reactors are available. Analytical equipment is in place.

Figure 7.1: The main laboratory of the Process group

Figure7. 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 (2012-2013)

Publications listed under PECxx-yy indicate CAPEC publications where one or more authors are CAPEC members, whether or not PROCESS is involved.

	A - Ph.D. Theses and Monographs
PEC12-40	Noor Asma Fazli Bin Abdul Samad, 2012, "Control of Process Operations and Monitoring of Product Qualities through Generic Model-based Framework in Crystallization Processes", Ph.D. thesis
PEC12-47 Book chp.	Gani, R., Gernaey, K. V. and Sin, G., 2012, "Process Systems Engineering, 1. Introduction", Ullmann's Encyclopedia of Industrial Chemistry, DOI: 10.1002/14356007.b06_317.pub2
PEC12-48 Book chp.	Gani, R., Cameron, I., Lucia, A., Sin, G. and Georgiadis, M., 2012, "Process Systems Engineering, 2. Modeling and Simulation", Ullmann's Encyclopedia of Industrial Chemistry, DOI: 10.1002/14356007.o22_o06
PEC12-49 Book chp.	Sin, G., Ghosh, K., Natarajan, S., Srinivasan, R., Adhitya, A., Karimi, I. A., Papadokonstantakis, S., Hungerbühler, K. and Angelo, P., 2012, "Process Systems Engineering, 7. Abnormal Events Management and Process Safety", Ullmann's Encyclopedia of Industrial Chemistry. DOI: 10.1002/14356007.o22_o11
PEC12-57 Book	Gani, R., Gernaey, K. V. and Sin, G., 2012, "Process Systems Engineering", in "Ullmann's Encyclopedia of Industrial Chemistry", Online ISBN: 9783527306732, DOI: 10.1002/14356007
PEC12-60	Azizul Azri Bin Mustaffa, **2013**, "Development and Analysis of Group Contribution^{Plus} Models for Property Prediction of Organic Chemical Systems", Ph.D. thesis
PEC13-14 Book Chp.	Rafiqul Gani, Mario R. Eden, TrulsGundersen, Michael C. Georgiadis, John. M. Woodley, Teresa López-Arenas, Mauricio Sales-Cruz, Eduardo S. Perez-Cisneros, Charles C. Solvason, Nishanth G. Chemmangattuvalappil, Mario R. Eden, Philip Lutze, Brock C. Roughton, Kyle V. Camarda, Elizabeth M. Topp, **2013**, "Process Systems Engineering, 4. Process and Product Synthesis, Design, and Analysis", Ullmann's Encyclopedia of Industrial Chemistry, DOI: 10.1002/14356007.o22_o08
PEC13-35	Naweed Al-Haque, **2013**, "Integrating Porous Resins in Enzymatic Processes", PhD. thesis

	B - Reviewed publications in International Journals
PEC10-42	Philip Lutze, Alicia Román-Martinez, John M. Woodley, Rafiqul Gani, 2012, "A systematic synthesis and design methodology to achieve process intensification in (bio) chemical processes", Computers & Chemical Engineering, 36, pp. 189-207
PEC10-43	E. Conte, R. Gani, Y. S. Cheng, K. M. Ng, 2012, "Design of Formulated Products: Experimental Component", AIChE Journal, 58(1), pp. 173-189
PEC11-06	Jakob Kjøbsted Huusom, Niels Kjølstad Poulsen, Sten Bay Jørgensen, John Bagterp Jørgensen, 2012, "Tuning SISO Offset-Free Model Predictive Control Based on ARX Models", Journal of Process Control, 22, pp. 1997-2007

PEC11-53	Martina Heitzig, Yunhong Rong, Christopher Gregson, Gürkan Sin, Rafiqul Gani, 2012, "Systematic Multi-scale Model Development Strategy for Fragrance Spraying Process and Transport", Chemical Engineering & Technology, 35(8), pp. 1381-1391
PEC11-54	Ricardo Morales-Rodriguez, A. S.Meyer, K. V.Gernaey, G. Sin, 2012, "A framework for model-based optimization of bioprocesses under uncertainty: Lignocellulosic ethanol production case", Computers and Chemical Engineering, 42, pp. 115-129
PEC11-55	Tiina M. Komulainen, RasmusEnemark-Rasmussen, Gürkan Sin, John P. Fletcher, David Cameron, 2012, "Experiences on dynamic simulation software in chemical engineering education", Education for Chemical Engineers journal, 7, pp. e153–e162
PEC11-56	Alberto Quaglia, Bent Sarup, Gürkan Sin, Rafiqul Gani, 2012, "Integrated Business and Engineering Framework for Synthesis and Design of Enterprise-Wide Processing Networks", Computers and Chemical Engineering, 38, pp. 213-223
PEC12-03	RomainPrivat, Elisa Conte, Jean-Noël Jaubert and Rafiqul Gani, 2012, "Are safe results obtained when SAFT equations are applied to ordinary chemicals? Part 2: study of solid-liquid equilibria in binary systems", Fluid Phase Equilibria, 318, pp. 61-76
PEC12-04	Prado-Rubio, O.A., Jørgensen, S.B. and Jonsson, G., 2012, "pH control structure design for a periodically operated membrane separation process", Computers and Chemical Engineering Journal, 43, pp. 120-129
PEC12-05	Amol Shivajirao Hukkerikar, Bent Sarup, Antoon Ten Kate, Jens Abildskov, Gürkan Sin, and Rafiqul Gani, 2012, "Group-contribution^{+} (GC^{+}) based estimation of properties of pure components: Improved property estimation and uncertainty analysis", Fluid Phase Equilibria, 321, pp. 25-43
PEC12-15	RasmusWedberg, Günther H. Peters, Jens Abildskov, 2012, "Protein Dynamics in Organic Media at Varying Water Activity Studied by Molecular Dynamics Simulation", J. Phys. Chem. B, 116(8), pp 2575–2585
PEC12-21	Jørgensen P.H., Thomsen K., Abildskov J., von Solms N.S., 2012, "Phase Equilibrium Modelling of Gas Hydrate Systems for CO_2 Capture", J. Chem. Thermodynamics, 48: 13-27
PEC12-26	Brock C. Roughton, Brianna Christian, John White, Kyle V. Camarda, and Rafiqul Gani, 2012, "Simultaneous Design of Ionic Liquid Entrainers and Energy Efficient Azeotropic Separation Processes", Computers and Chemical Engineering Journal, 42, pp. 248-262
PEC12-27	Zhihong Yuan, Bingzhen Chen, Gürkan Sin, Rafiqul Gani, 2012, "State-of-the-Art and Progress in the Optimization based Simultaneous Design and Control for Chemical Processes", AIChE Journal, 58(6), pp. 1640-1659
PEC12-28	Vangsgaard, A.K., Mauricio-Iglesias, M., Gernaey, K.V., Smets, B.F. & Sin, G., 2012, "Sensitivity analysis of autotrophic N removal by a granule based bioreactor: Influence of mass transfer versus microbial kinetics", Bioresource Technology, 123, pp. 230-241
PEC12-29	Mauricio-Iglesias, M. Huusom, J. K. Sin, G., **2013**, "Control assessment for heat integrated systems. An industrial case study for ethanol recovery", Chemical Engineering and Processing: Process Intensification, 67, pp. 60-70
PEC12-31	Noor Asma Fazli Bin Abdul Samad, Gürkan Sin, Krist V Gernaey, Rafiqul Gani, **2013**, "A systematic framework for design of process monitoring and control (PAT) systems for crystallization processes", Computers & Chemical Engineering, 54, pp. 8-23
PEC12-35	Albert E. Cervere-Radrell, Tommy Skovby, Søren Kiil, Rafiqul Gani, Krist V. Gernaey, 2012, "Active pharmaceutical ingredient (API) production involving continous processes – A PSE-assisted design framework", European Journal of Pharmaceutics and Biopharmaceutics, 82(2), pp. 437-456

PEC12-36	Naweed Al-Haque, Paloma A. Santacoloma, Watson Neto, Pär Tufvesson, Rafiqul Gani and John M. Woodley, 2012, "A robust methodology for kinetic model parameter estimation for biocatalytic reactions", Biotechnol. Prog., 28(5), pp. 1186-1196
PEC12-37	Jose Manuel Roman Marin, Jakob Kjøbsted Huusom, Nicolas Javier Alvarez, Qian Huang, Henrik Koblitz Rasmussen, Anders Bach, Anne Ladegaard Skov, Ole Hassager, **2013**, "A control scheme for filament stretching rheometers with application to polymer melts", Journal of Non-Newtonian Fluid Mechanics, Vol. 194, pp. 14-22
PEC12-39	Abildskov J., van Leeuwen M.B., Boeriu C.G., van den Broek L.A.M., **2013**, "Computer-Aided Solvent Screening for Biocatalysis", J. Mol. Cat. B: Enzymatic, 85-86: pp. 200-213
PEC12-41	V. Ibarra-Junquera, S.B. Jørgensen, J.J. Virgen-Ortíz, P. Escalante-Minakata, J.A. Osuna-Castro, 2012, "Following an Optimal Batch Bioreactor Operations Model", Chemical Engineering & Processing: Process Intensification, Vol. 62, pp. 114-128
PEC12-46	Alberto Quaglia, Bent Sarup, Gürkan Sin, Rafiqul Gani, **2013**, "A systematic framework for enterprise-wide optimization: Synthesis and design of processing network under uncertainty", Computers and Chemical Engineering, In Press, DOI: http://dx.doi.org/10.1016/j.compchemeng.2013.03.018
PEC12-50	Zhihong Yuan, Bingzhen Chen, Rafiqul Gani, **2013**, "Applications of Process Synthesis: Moving from Conventional Chemical Processes towards Biorefinery Processes", Computers and Chemical Engineering, Vol. 49, pp. 217-229
PEC12-51	Amol Hukkerikar, Sawitree Kalakul, Bent Sarup, Douglas M. Young, Gürkan Sin, Rafiqul Gani, 2012, "Estimation of environment-related properties of chemicals for design of sustainable processes: Development of group-contribution^{+} (GC^{+}) models and uncertainty analysis", Journal of Chemical Information and Modeling, 52(11), pp. 2823-2839
PEC12-53	Philip Lutze, Deenesh K. Babi, John M. Woodley, Rafiqul Gani, **2013**, "Phenomena Based Methodology for Process Synthesis Incorporating Process Intensification", Industrial & Engineering Chemistry Research, In Pres, DOI: 10.1021/ie302513y
PEC12-54	Lida Simasatitkul, Amornchai Arpornwichanop and Rafiqul Gani, **2013**, "Design methodology for bio-based processing: Biodiesel and fatty alcohol production", Computers & Chemical Engineering, In Press, DOI: http://dx.doi.org/10.1016/j.compchemeng.2013.01.018
PEC12-55	Ana Carvalho, Henrique A. Matos, Rafiqul Gani, **2013**, "SustainPro - A tool for systematic process analysis, generation and evaluation of sustainable design alternatives", Computers & Chemical Engineering, Vol. 50, pp. 8-27
PEC12-56	Roberta Ceriani, Rafiqul Gani, Y.A. Liu, **2013**, "Prediction of vapor pressure and heats of vaporization of edible oil/fat compounds by group contribution", Fluid Phase Equilibria, 337, pp. 53-59
PEC12-62	Vladimir Diky, Robert Dennis Chirico, Chris Muzny, Andrei Kazakov, Kenneth Kroenlein, Joseph W. Magee, IlmutdinAbdulagatov, Jeong Won Kang, Rafiqul Gani, and Michael Frenkel, **2013**, "ThermoData Engine (TDE): Software Implementation of theDynamic Data Evaluation Concept. 8. Properties of Material Streams and Solvent Design", Journal of Chemical Information and Modelling, 53, 249−266
PEC13-01	S. Sansonetti, T.J. Hobley, S. Curcio, J. Villadsen, G. Sin, **2013**, "Use of continuous lactose fermentation for ethanol production by *Kluveromycesmarxianus*for verification and extension of a biochemically structured model", Bioresource Technology, DOI: http://dx.doi.org/10.1016/j.biortech.2012.12.080
PEC13-03	Lind Morten, Yoshikawa Hidekazu, Jørgensen Sten Bay, Yang Ming, 2012, "Modeling operating modes for the MONJU nuclear power plant", International Journal Nuclear Safety, 3, pp. 314-324

PEC13-11	Gürkan Sin, Rafiqul Gani, Kim Dam-Johansen, **2013**, ”Denmark’s Chemicals Industry: Progress and Challenges”, Chemical Engineering Progress (CEP: February 2013), American Institute of Chemical Engineers (AIChE), pp. 54-59
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, Accepted, DOI: 10.1002/jctb.4060
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 Sci. Technol., Accepted., DOI:10.2166/wst.2013.174
PEC12-52	Larissa P Cunico, Amol S Hukkerikar, Roberta Ceriani, Bent Sarup, Rafiqul Gani, 2013, “Molecular Structure-Based Methods of Property Prediction in Application to Lipids: A Review and Refinement”, Fluid Phase Equilibria, http://dx.doi.org/10.1016/j.fluid.2013.04.004
PEC13-12	Eric Lueshen, Martina Heitzig, Gurkan Sin, Rafiqul Gani and Andreas Linniger, **2013**, “First Principles Pharmacokinetic Modeling; A Quantitative Study on Cyclosporin”, Computers and Chemical Engineering, 54, pp 97-110

	C - In press/Submitted Manuscripts
PEC12-43	Daniel HaugaardOlesen, Jakob Kjøbsted Huusom, John Bagterp Jørgensen, **2013**, ”Tuning Procedure for ARX-based MPC of Multivariate Processes”, Proceedings of American Control Conference (ACC), Accepted
PEC12-61 Book Chp.	Michele Mattei, Elisa Conte, Georgios M. Kontogeorgis, Rafiqul Gani, **2013**, “Prediction of thermo-physical properties of liquid formulated products”, in “Product Design” (Editors: V. Broeckel, D. Wagner, W. Meier), Wiley, In Press
PEC13-02	Noor Asma Fazli Abdul Samad, Gürkan Sin, Krist V Gernaey, Rafiqul Gani, **2013**, ”Introducing Uncertainty Analysis of Nucleation and Crystal Growth Models in Process Analytical Technology (PAT) System Design of Crystallization Processes”, European Journal of Pharmaceutics and Biopharmaceutics, Submitted
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, In Press
PEC13-05	Nor Alafiza Yunusa, Krist V. Gernaeya, John M. Woodleya and Rafiqul Gani, **2013**, “Design of Sustainable Blended Products using an Integrated Methodology”, Computer-Aided Chemical Engineering Series, Volume 32, In Press
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, In Press
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, In Press

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, In Press
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, In Press
PEC13-10	Thomas Bisgaard, Jakob Kjøbsted Huusom, Jens Abildskov, **2013**, "Dynamic effects of diabatization in distillation columns", Computer-Aided Chemical Engineering Series, Volume 32, In Press
PEC13-16	Philip Lutze, Rafiqul Gani, **2013**, "Process intensification in integrated membrane processes", Book chapter in Alfredo Cassano and Enrico Drioli: Integrated Membrane Operations, In Press
PEC13-19	Remus MihailPrunescu, Jakob Munch Jensen, MogensBlanke and Gürkan Sin, **2013**, "Modelling and L1 Adaptive Control of pH in Bioethanol Enzymatic Process", Proceedings of 2013 American Control Conference (ACC), In Press
PEC13-21	Jing Wu, Laibin Zhang, Morten Lind, Wei Liang, Jinqiu Hu, Sten Bay Jørgensen, Gürkan Sin, Zia UllahKhokhar, **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), Submitted
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), Submitted
PEC13-23	Singh, Ravendra; Godfrey, Andy; Gregertsen, Bjorn; Muller, Frans, Vankayala, Bhanu; Hass-Santo, Katja; Gernaey, Krist; Gani, Rafiqul; Woodley, John, **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
PEC13-26	Ravendra Singh, Andy Godfrey, BjörnGregertsen, Frans Muller, Krist V Gernaey, Rafiqul Gani, John M Woodley, **2013**, "Systematic substrate adoption methodology (SAM) for future flexible, generic pharmaceutical production processes", Computers and Chemical Engineering, Submitted
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), Accepted
PEC13-28	Saranya Mangnimit, PomthongMalakul, and Rafiqul Gani, **2013**, "Sustainablbe Process Design of Lignocellulose based Biofuel", Proceedings of WCCE9, Accpeted
PEC13-29	Sawitree Kalakul, PomthongMalakul, KitipatSiemanond, 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), Accepted
PEC13-30	Sawitree Kalakul, PomthongMalakul, KitipatSiemanond, Rafigul Gani, 2013, "A Generic Life Cycle Assessment Tool For Chemical-biochemical Processes", Proceedings of WCCE9 &APCChE 2013, Accepted
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 CAB (Computer Applications in Biotechnology), Submitted

PEC13-32	Mauricio-Iglesias, M. Montero-Castro, I. Mollerup, A.L. Sin, G., **2013**, "Self-optimising control of sewer systems", Proceedings of DYCOPS (Dynamics and Control of Process Systems), Submitted
PEC13-33	Jason Price, Mathias Nordblad, John M. Woodley, Jakob K. Huusom, **2013**, "Application of Uncertainty and SensitivityAnalysisto a KineticModelforEnzymatic Biodiesel Production", Proceedings of CAB (Computer Applications in Biotechnology), Submitted
PEC13-34	Thomas Bisgaard, Jakob Kjøbsted Huusom and Jens Abildskov, **2013**, "A Modeling Framework for Conventional and Heat Integrated Distillation Columns", 10th IFAC International Symposium on Dynamics and Control of Process Systems, Submitted

	D - Reviewed Conference Proceedings
PEC11-52	Nor Alafiza Yunus, Krist V Gernaey, John M Woodley & Rafiqul Gani, 2012, "Computer-aided approach for design of tailor-made blended products", Proceedings of the 3rd International Gas Processing Symposium, Editors: AbdelwahabAroussi and FaridBenyahia, pp. 303-310
PEC11-57	Alberto Quaglia, Bent Sarup, Gürkan Sin, Rafiqul Gani, 2012, "Synthesis and Design of Processing Networks: Stochastic Formulation and Solution", Computer-Aided Chemical Engineering Series, Volume 30, pp. 467-471
PEC12-02	Mauricio-Iglesias, M., Jørgensen, S.B. Sin, G., 2012, "A systematic methodology for controller tuning in wastewater treatment plants", IFAC Proceedings Volumes (IFAC-PapersOnline) 8 (PART 1), pp. 828-833
PEC12-06	Nor Alafiza Yunus, Krist V. Gernaey, John M. Woodley and Rafiqul Gani, 2012, "An Integrated Methodology for Design of Tailor-Made Blended Products", Computer-Aided Chemical Engineering Series, Volume 30, pp. 752-756
PEC12-07	Noor Asma Fazli Abdul Samad, Kresten Troelstrup Meisler, Gürkan Sin, Krist V. Gernaey, Rafiqul Gani, 2012, "A Generic Framework for Systematic Design of Process Monitoring and Control System for Crystallization Processes", 22nd European Symposium on Computer Aided Process Engineering, ESCAPE22, (only on CD)
PEC12-08	Igor Mitrofanov, Sascha Sansonetti, Jens Abildskov, Gürkan Sin and Rafiqul Gani, 2012, "The Solvent Selection framework: solvents for organic synthesis, separation processes and ionic-liquids solvents", Computer-Aided Chemical Engineering Series, Volume 30, pp. 762-766
PEC12-09	Amol Hukkerikar, Mark Jones, Bent Sarup, Jens Abildskov, Gürkan Sin, and Rafiqul Gani, 2012, "Sensitivity of Process Design due to Uncertainties in Property Estimates", Computer-Aided Chemical Engineering, Vol 31, pp. 200-204(PSE-2012)
PEC12-10	RasmusEnemark-Rasmussen, David Cameron, Per Bagge Angeloand Gürkan Sin, 2012, "A simulation based engineering method to support HAZOP studies", Computer-Aided Chemical Engineering, Vol 31, pp. 1271-1275(PSE-2012)
PEC12-11	LidaSimasatitkul, AmornchaiArpornwichanop, Rafiqul Gani, 2012, "Design methodology for bio-based processing: Biodiesel and fatty alcohol production", Computer-Aided Chemical Engineering, Vol 31, pp. 855-859(PSE-2012)
PEC12-12	Chiara Piccolo, Andrew Shaw, George Hodges, Patrick M. Piccione, John P. O'Connell, Rafiqul Gani, 2012, "A framework for the design of reacting systems with phase transfer catalysis", Computer-Aided Chemical Engineering Series, Volume 30, pp. 757-761
PEC12-13	Michele Mattei, Georgios M. Kontogeorgis, Rafiqul Gani, 2012, "A Systematic Methodology for Design of Emulsion Based Chemical Products", Computer-Aided Chemical Engineering, Vol, 31, pp. 220-224(PSE-2012)

PEC12-16	Philip Lutze, Deenesh K. Babi, John Woodley, Rafiqul Gani, 2012, "Phenomena-based Process Synthesis and Design to achieve Process Intensification", Computer-Aided Chemical Engineering, Vol, 31, pp. 1697-1701
PEC12-17	Ravendra Singh, Raquel Rozada-Sanchez, William Dean, Jacob Perkins, Frans Muller, Andy Godfrey, Krist V. Gernaey, Rafiqul Gani, John M. Woodley, 2012, "A generic process template for continuous pharmaceutical production", Computer-Aided Chemical Engineering, Vol, 31, pp. 715-719(PSE-2012)
PEC12-19	Guofeng Zhou, John Bagterp Jørgensen, Christophe Duwig, Jakob Kjøbsted Huusom, 2012, "State Estimation in the Automotive SCR DeNOx Process", Proceedings of The International Symposium on Advanced Control of Chemical Processes (AdChem 12), pp. 501-506
PEC12-20	Noor Asma Fazli Abdul Samad, Kresten Troelstrup Meisler, Krist V. Gernaey, Nicolas Smit von Solms, Rafiqul Gani, 2012, "Systematic identification of crystallization kinetics within a generic modelling framework", Computer-Aided Chemical Engineering, Vol, 31, pp. 945-949(PSE-2012)
PEC12-32	Anna Katrine Vangsgaard, A. GizemMutlu, Krist V. Gernaey, Barth F. Smets, Gürkan Sin, 2012, "Calibration and validation of a model describing complete autotrophic nitrogen removal in granular sludge", proceedings of IWA Nutrient Removal and Recovery 2012: Trends in NRR, pp. 193-194
PEC12-33	Anna Katrine Vangsgaard, Miguel Mauricio-Iglesias, Borja Valverde Pérez, Krist V. Gernaey, Gürkan Sin, 2012, "pH variation and influence in a nitrogen converting biofilm dominated by autotrophs", proceedings of IWA Nutrient Removal and Recovery 2012: Trends in NRR, pp. 15-16
PEC12-34	A.G. Mutlu, A.K. Vangsgaard, G. Sin, B.F. Smets, 2012, "An operation protocol for facilitating start-up of single-stage autotrophic nitrogen removing reactors based on process stoichiometry", proceedings of IWA World Water Congress & Exhibition, IWA-8145
PEC12-38	X. Flores-Alsina, J. Guerrero, A.-K.Vangsgaard, A.Guisasola, J.Baeza, U.Jeppsson, B.F.Smets, G.Sin, K.V.Gernaey, 2012, "Recent trends in modelling and simulation of nutrient removal systems", proceedings of IWA Nutrient Removal and Recovery 2012: Trends in NRR, pp. 29-32
PEC12-42	Thomas Bisgaard, Jakob Kjøbsted Huusom and Jens Abildskov, 2012, "Dynamic Effects of Diabatization in Distillation Columns", Electronic Proceedings of the 10th European Workshop on Advanced Control and Diagnosis (ACD 2012), Paper no. 24
PEC12-44	Daniel Olesen, Jakob Kjøbsted Huusom and John Bagterp Jørgensen, 2012, "Optimization based tuning approach for offset free MPC", Electronic Proceedings of the 10th European Workshop on Advanced Control and Diagnosis (ACD 2012), Paper no. 40
PEC12-59	Mauricio-Iglesias, M. Valverde-Pérez, B. Sin, G., 2012, "Incremental design of control system of SHARON-Anammox process for autotrophic nitrogen removal", Electronic Proceedings of the 10th European Workshop on Advanced Control and Diagnosis (ACD 2012)

	E - Other Publications & Reports
PEC11-50	Rafiqul Gani, 2012, "A systems engineering approach to manage the complexity in sustainable chemical product-process design", electronic unreviewed proceedings to 13th Industrialist's Conference, info on USB stick
PEC11-51	Sin Gürkan, 2012, "An integrated knowledge-based framework for synthesis and design of enterprise-wide processing networks", electronic unreviewed proceedings to 13th Industrialist's Conference, info on USB stick

	Valverde-Pérez, B. Mauricio-Iglesias, M. Sin, G., 2012, ”Modelling and control design for SHARON/Anammox reactor sequence”, Proceedings of Nordic Process and Control Workshop 17 (NPCW17), Technical University of Denmark, KgsLyngby, Denmark, pp. 176-184
	Ane H. Mollerup, M. Mauricio-Iglesias, N. B. Johansen, D. Thornberg, P. S. Mikkelsen and G. Sin, 2012, “Model-based analysis of control performance in sewer systems”, Proceedings of Nordic Process and Control Workshop 17 (NPCW17), Technical University of Denmark, KgsLyngby, Denmark, pp. 123-127
	Prado-Rubio, O.A., Jørgensen, S.B. and Jonsson, 2012, “On controllability of an integrated bioreactor and periodically operated membrane separation process”, Proceedings of Nordic Process and Control Workshop 17 (NPCW17), Technical University of Denmark, KgsLyngby, Denmark, p. 207
	Remus M. Prunescu, MogensBlanke, Jakob M. Jensen, Gürkan Sin, 2012, “Temperature Modelling of the Biomass Pretreatment Process”, Proceedings of the 17th Nordic Process Control Workshop (NPCW17), Technical University of Denmark, KgsLyngby, Denmark pp. 8-17
	Sten Bay Jørgensen and Morten Lind, 2012, “Modeling Operating Modes during Plant Life Cycle”, Proceedings of the 17th Nordic Process Control Workshop (NPCW17), Technical University of Denmark, KgsLyngby, Denmark p. 60
	Mads O. Albaek, Krist V. Gernaey, Morten S. Hansen, Stuart M. Stocks, 2012, “Modelling Fungal Fermentations For Enzyme Production”, Proceedings of the 17th Nordic Process Control Workshop (NPCW17), Technical University of Denmark, KgsLyngby, Denmark, p. 185
	Jason A. Price, Jakob Kjøbsted Huusom, Mathias Nordblad, John Woodley, 2012, “Operation and Control of Enzymatic Biodiesel Production”, Proceedings of the 17th Nordic Process Control Workshop (NPCW17), Technical University of Denmark, KgsLyngby, Denmark, pp. 186
	Guofeng Zhou, Jakob K. Huusom, John Bagterp Jørgensen, 2012, “State Estimation for the Automotive SCR Process”, Proceedings of the 17th Nordic Process Control Workshop (NPCW17), Technical University of Denmark, KgsLyngby, Denmark, p. 204
PEC12-14	Valverde-Pérez, B., Mauricio-Iglesias, M., Sin, G., 2012, “Control of SHARON reactor for autotrophic nitrogen removal in two-reactor configuration”, Unreviewed article in proceedings of EcoTechnologies for Wastewater Treatment 2012 IWA International Conference, ISBN-978-84-695-3605-6
PEC12-18	Amol Hukkerikar, Bent Sarup, Jens Abildskov, Gürkan Sin, and Rafiqul Gani, 2012, ”Development of property models with uncertainty estimate for reliable product-process design”, Proceedings of Industrial Use of Molecular Thermodynamics (InMoTher 2012), p. 43
PEC12-25	Rafiqul Gani and John Woodley, 2012, “CAPEC-PROCESS Research Report 2012”, CAPEC-PROCESS Internal Report, DTU-KT, Lyngby, Denmark
PEC12-30	Azizul Azri Mustaffa, Georgios Kontogeorgis, Rafiqul Gani, 2012, ”Application of the UNIFAC-CI Model for Phase Equilibria Predictions of Organic Chemical System”, Industrial Use of Molecular Thermodynamics (InMoTher 2012), p. 65
PEC12-45	Anna Katrine Vangsgaard, Krist V. Gernaey, Gürkan Sin og A. Gizem Mutlu, 2012, ”Energibesparende biologisk proces til kvælstoffjernelse i spildevand”, Dansk Kemi, 93(10), pp. 16-18
PEC13-25	Rafiqul Gani and John Woodley, 2013, “CAPEC-PROCESS Research Report 2013”, CAPEC-PROCESS Internal Report, DTU-KT, Lyngby, Denmark

	F - Conference Presentations 2012
2012-1	Rafiqul Gani, 2012, "A systems engineering approach to manage the complexity in sustainable chemical product-process design", 13th Industrialist's Conference, Riyadh, Saudi Arabia, 17-19 January, **Invited**
2012-2	Sin Gürkan, 2012, "An integrated knowledge-based framework for synthesis and design of enterprise-wide processing networks", 13th Industrialist's Conference, Riyadh, Saudi Arabia, 17-19 January, **Invited**
2012-3	Rodríguez-Valverde, B. Mauricio-Iglesias, M. Sin, G., 2012, "A systematic methodology for controller tuning in wastewater treatment plants", Nordic Process and Control Workshop 17 (NPCW17), Lyngby, Denmark, 25-27 January
2012-4	Ane H. Mollerup, M. Mauricio-Iglesias, N. B. Johansen, D. Thornberg, P. S. Mikkelsen and G. Sin, 2012, "Model-based analysis of control performance in sewer systems", Nordic Process and Control Workshop 17 (NPCW17), Lyngby, Denmark, 25-27 January
2012-5 Poster	Prado-Rubio, O.A., Jørgensen, S.B. and Jonsson, 2012, "On controllability of an integrated bioreactor and periodically operated membrane separation process", Nordic Process and Control Workshop 17 (NPCW17), Lyngby, Denmark, 25-27 January
2012-6	Remus M. Prunescu, MogensBlanke, Jakob M. Jensen, Gürkan Sin, 2012, "Temperature Modelling of the Biomass Pretreatment Process", Proceedings of the 17th Nordic Process Control Workshop (NPCW17), Technical University of Denmark, KgsLyngby, Denmark, 25-27 January
2012-7	Sten Bay Jørgensen and Morten Lind, 2012, "Modeling Operating Modes during Plant Life Cycle", Proceedings of the 17th Nordic Process Control Workshop (NPCW17), Technical University of Denmark, KgsLyngby, Denmark, 25-27 January
2012-8 Poster	Jason A. Price, Jakob Kjøbsted Huusom, Mathias Nordblad, John Woodley, 2012, "Operation and Control of Enzymatic Biodiesel Production", Proceedings of the 17th Nordic Process Control Workshop (NPCW17), Technical University of Denmark, KgsLyngby, Denmark, 25-27 January
2012-9 Poster	Guofeng Zhou, Jakob K. Huusom, John Bagterp Jørgensen, 2012, "State Estimation for the Automotive SCR Process", Proceedings of the 17th Nordic Process Control Workshop (NPCW17), Technical University of Denmark, KgsLyngby, Denmark, 25-27 January
2012-10	Rafiqul Gani, 2012, "A model-data based systems approach to process intensification", Inaugural scientific conference: Process Technology For The Future World – Building Bridges Across Boundaries, TU Delft Process Technology Institute, Delft, The Netherlands, 2 March, **Plenary Lecture**
2012-11 Oral pres.	Nor Alafiza Yunus, Krist V Gernaey, John M Woodley & Rafiqul Gani, 2012, "Computer-aided approach for design of tailor-made blended products", 3rd International Gas Processing Symposium, Doha, Qatar, 5-7 March
2012-12 Poster	Azizul Azri Mustaffa, Georgios Kontogeorgis, Rafiqul Gani, 2012, "Application of the UNIFAC-CI Model for Phase Equilibria Predictions of Organic Chemical System", Industrial Use of Molecular Thermodynamics (InMoTher 2012), Lyon, France, 19-20 March
2012-13	Amol Hukkerikar, Bent Sarup, Jens Abildskov, Gürkan Sin, and Rafiqul Gani, 2012, "Development of property models with uncertainty estimate for reliable product-process design", Industrial Use of Molecular Thermodynamics (InMoTher 2012), Lyon, France, 19-20 March
2012-14	Noor Asma Fazli Abdul Samad, Kresten T. Meisler, Gürkan Sin, Krist V. Gernaey and Rafiqul Gani, 2012, "Quantifying uncertainties of nucleation and crystal growth models on PAT system performance for crystallization processes", Advances in Process Analytics and Control Technology (APACT-12), Newcastle UK, 25-27 April

2012-15 Poster	Noor Asma Fazli Abdul Samad, Kresten T. Meisler, Krist V. Gernaey, Nicolas von Solms and Rafiqul Gani, 2012, "Framework for the analysis of crystallization operations", Advances in Process Analytics and Control Technology (APACT-12), Newcastle UK, 25-27 April
2012-16	Rafiqul Gani, 2012, "A model-data based systems approach to process intensification", The Mexican Academy for Research and Teaching in Chemical Engineering (AMIDIQ), San Jose del Cabo, BCS, Mexico, 1-4 May, **Plenary lecture**
2012-17	Sten Bay Jørgensen, 2012, "Integrating process and automation design based on functional concepts", invited talk at Morten Lind Professor Emeritus Seminar, DTU, Lyngby, Denmark, 14 May, **Invited Talk**
2012-18 Poster	Alberto Quaglia, Bent Sarup, Gürkan Sin, Rafiqul Gani, 2012, "Synthesis and Design of Processing Networks: Stochastic Formulation and Solution", ESCAPE22, London, UK, 17-20 June
2012-19 Poster	Nor Alafiza Yunus, Krist V. Gernaey, John M. Woodley and Rafiqul Gani, 2012, "An Integrated Methodology for Design of Tailor-Made Blended Products", ESCAPE22, London, UK, 17-20 June
2012-20	Noor Asma Fazli Abdul Samad, Kresten Troelstrup Meisler, Gürkan Sin, Krist V. Gernaey, Rafiqul Gani, 2012, "A Generic Framework for Systematic Design of Process Monitoring and Control System for Crystallization Processes", ESCAPE22, London, UK, 17-20 June
2012-21 Poster	Igor Mitrofanov, Sascha Sansonetti, Jens Abildskov, Gürkan Sin and Rafiqul Gani, 2012, "The Solvent Selection framework: solvents for organic synthesis, separation processes and ionic-liquids solvents", ESCAPE22, London, UK, 17-20 June
2012-22 Poster	Chiara Piccolo, Andrew Shaw, George Hodges, Patrick M. Piccione, John P. O'Connell, Rafiqul Gani, 2012, "A framework for the design of reacting systems with phase transfer catalysis", ESCAPE22, London, UK, 17-20 June
2012-23	Azizul Azri Mustaffa, Georgios Kontogeorgis, Jeong Won Kang, Rafiqul Gani, 2012, "Development and Analysis of Original UNIFAC-CI and Modified UNIFAC-CI Models for Prediction of VLE and SLE Systems", 18th Symposium on Thermophysical Properties, Boulder, CO, USA, 24-29 June
2012-24	Amol Shivajirao Hukkerikar, Bent Sarup, Jens Abildskov, Gürkan Sin, and Rafiqul Gani, 2012, "Estimation of Properties of Pure Components Using Improved Group-Contribution+ (GC+) Based Models and Uncertainty Analysis", 18th Symposium on Thermophysical Properties, Boulder, CO, USA, 24-29 June
2012-25	Amol Hukkerikar, Mark Jones, Gürkan Sin, Rafiqul Gani, 2012, "Effect of Uncertainties in Physical Property Estimates on Process Design - Sensitivity Analysis", 18th Symposium on Thermophysical Properties, Boulder, CO, USA, 24-29 June
2012-26	Vladimir V. Diky, Robert D. Chirico, Chris D. Muzny, Andrei F. Kazakov, Kenneth Kroenlein, Joseph W. Magee, Ilmutdin M. Abdulagatov, Carlos Axel Diaz-Tovar, Jeong Won Kang, Rafiqul Gani, Michael Frenkel, 2012, "NIST ThermoData Engine: Extension to Solvent Design and Propagation of Uncertainties for Process Simulation", 18th Symposium on Thermophysical Properties, Boulder, CO, USA, 24-29 June
2012-27	Rafiqul Gani and Sascha Sansonetti, 2012, "Property Modelling and Databases in Product-Process Design", 18th Symposium on Thermophysical Properties, Boulder, CO, USA, 24-29 June, **Invited Keynote Lecture**
2012-28	Babi DK, Lutze P, Woodley JM and Gani R, 2012, "Achieving process intensification form the application of a phenomena based synthesis, Design and intensification methodology", ANQUE ICCE 2012, Sevilla, Spain, 24-27 June

2012-29	Pennati A., Quaglia A., Sin G. and Gani R., 2012, ”Synthesis of Industrial Water Networks”, ANQUE ICCE 2012, Sevilla, Spain, 24-27 June
2012-30 Poster	Ballesteros, E,; Gani, R.;Sin, G., 2012, "Separation of azeotropic mixtures", ANQUE ICCE 2012, Sevilla, Spain, 24-27 June
2012-31	Rafiqul Gani, 2012, “A New Paradigm for Chemical Engineering?”, ANQUE ICCE 2012, Sevilla, Spain, 24-27 June, **Invited plenary lecture**
2012-32 Poster	Valverde-Pérez, B., Mauricio-Iglesias, M., Sin, G., 2012, “Control of SHARON reactor forautotrophicnitrogenremoval in two-reactor configuration”, EcoTechnologies for Wastewater Treatment, organised by the IWA (International Water Association), Santiago de Compostela, Spain, 25-27 June
2012-33	Mauricio-Iglesias, M., Jørgensen, S.B. Sin, G., 2012, “A systematic methodology for controller tuning in wastewater treatment plants”,The International Symposium on Advanced Control of Chemical Processes (AdChem), Singapore, 10-13 July
2012-34 Poster	Guofeng Zhou, John Bagterp Jørgensen, Christophe Duwig, Jakob Kjøbsted Huusom, 2012, “State Estimation in the Automotive SCR DeNOx Process”, The International Symposium on Advanced Control of Chemical Processes (AdChem), Singapore, 10-13 July
2012-35	RasmusEnemark-Rasmussen, David Cameron, Per Bagge Angelo and Gürkan Sin, 2012, “A simulation based engineering method to support HAZOP studies”, 11th International Symposium on Process Systems Engineering conference (PSE 2012), Singapore, 15-19 July
2012-36 Poster	Amol Hukkerikar, Mark Jones, Bent Sarup, Jens Abildskov, Gürkan Sin, Rafiqul Gani, 2012, “Sensitivity of Process Design due to Uncertainties in Property Estimates”, 11th International Symposium on Process Systems Engineering conference (PSE 2012), Singapore, 15-19 July
2012-37	LidaSimasatitkul, AmornchaiArpornwichanop, and Rafiqul Gani, 2012, “Design methodology for bio-based processing: Biodiesel and fatty alcohol production”, 11th International Symposium on Process Systems Engineering conference (PSE 2012), Singapore, 15-19 July
2012-38 Poster	Michele Mattei, Georgios M Kontogeorgis, Rafiqul Gani, 2012, “A Systematic Methodology for Design of Emulsion Based Chemical Products”, 11th International Symposium on Process Systems Engineering conference (PSE 2012), Singapore, 15-19 July
2012-39	Philip Lutze, Deenesh K. Babi, John Woodley, Rafiqul Gani, 2012, “Phenomena-based Process Synthesis and Design to achieve Process Intensification”, 11th International Symposium on Process Systems Engineering conference (PSE 2012), Singapore, 15-19 July
2012-40 Poster	Ravendra Singh, Raquel Rozada-Sanchez, William Dean, Jacob Perkins, Frans Muller, Andy Godfrey, Krist V. Gernaey, Rafiqul Gani, John M. Woodley, 2012, “A generic process template for continuous pharmaceutical production”, 11th International Symposium on Process Systems Engineering conference (PSE 2012), Singapore, 15-19 July
2012-41	Noor Asma Fazli Abdul Samad, Kresten Troelstrup Meisler, Krist V. Gernaey, Nicolas Smit von Solms, Rafiqul Gani, 2012, “Systematic identification of crystallization kinetics within a generic modelling framework”, 11th International Symposium on Process Systems Engineering conference (PSE 2012), Singapore, 15-19 July
2012-42	Vladimir Diky, Chirico Rd, Muzny CD, Kazakov A, Abdulagatov I, Magee JW, Kang JW, Gani R, Frenkel M, 2012, “ThermoData Engine: Extension to Solvent Design and Multi-component Process Stream Property Calculations with Uncertainty Analysis”, 22ndInternacioal Conference on Chemical Thermodynamics, ICCT 2012, Búzios, RJ, Brazil, 5-10 August

2012-43	Rafiqul Gani, 2012, "Modelling of physical properties – databases, uncertainties and predictive power", 22nd Internacioal Conference on Chemical Thermodynamics, ICCT 2012, Búzios, RJ, Brazil, 5-10 August, **Invited Plenary Lecture**
2012-44 Poster	Mutlu, A. G., Vangsgaard,A. K., JensenM. M., Smets B. F., 2012, "Architecture evolution of biomass aggregates in single stage nitritation/anammox reactors", 14th International Symposium on Microbial Ecology - ISME14, Copenhagen, Denmark, 19-24 August
2012-45	M. Jones, A. Hukkerikar, G. Sin, R. Gani, 2012, "Sensitivity of process design to uncertainties in property estimates applied to extractive distillation", CHISA-2012, Prague, Czech Republic, 25-29 August
2012-46	A. Quaglia, B. Sarup, G. Sin, R. Gani, 2012, "Synthesis and design of processing networks: decision making under uncertainty and sensitivity analysis", CHISA-2012, Prague, Czech Republic, 25-29 August
2012-47	I. Mitrofanov, J. Abildskov, G. Sin, and R. Gani, 2012, "Extension of computer aided solvent selection and design framework – organic solvents for phase transfer catalysis and solvent selection and solvent mixture design for pharmaceutical applications", CHISA-2012, Prague, Czech Republic, 25-29 August
2012-48	Sin, G., 2012, "Advanced sensitivity and uncertainty analysis for computer-aided process engineering", CHISA-2012, Prague, Czech Republic, 25-29 August, **Keynote Lecture**
2012-49	Mutlu, A.G., Vangsgaard, A.K., Smets, B.F. & Sin, G., 2012, "An operation protocol for facilitating start-up of single-stage autotrophic nitrogen removing reactors based on process stoichiometry", IWA World Water Congress & Exhibition, Busan, South Korea, 16-21 September
2012-50	Vangsgaard, A.K., Mutlu, A.G., Gernaey, K.V., Smets, B.F. & Sin, G., 2012, "Calibration and validation of model describing complete autotrophic nitrogen removal in granular sludge", IWA Nutrient Removal and Recovery 2012: Trends in NRR, 23-25 September 2012, Harbin, China
2012-51 Poster	Anna Katrine Vangsgaard, Miguel Mauricio-Iglesias, Borja Valverde-Pérez, Krist V. Gernaey, and Gürkan Sin, 2012, "pH variation and influence in an autotrophic nitrogen removing biofilm system: An efficient numerical solution strategy", IWA Nutrient Removal and Recovery 2012: Trends in NRR, 23-25 September 2012, Harbin, China
2012-52 Poster	Flores-Alsina X., Guerrero J., Vangsgaard A. K., Guisasola A., Baeza J., Jeppsson U., Smets B.F., Sin G., Gernaey K.V., 2012, "Recent trends in modelling and simulation of biological nutrient removal systems", IWA Nutrient Removal and Recovery 2012: Trends in NRR, Harbin, China, 23-25 September
2012-53	Larissa P. Cunico, Roberta Ceriani, Bent Sarup, Rafiqul Gani, 2012, "Consistent Prediction of Properties of Systems with Lipids", ESAT 2012, Berlin, Germany, 6-10 October
2012-54	Larissa P. Cunico, Amol S. Hukkerikar, Gürkan Sin, Rafiqul Gani, 2012, "Molecular structure based physical properties modelling", MTMS'12 (6th International Symposium on Molecular Thermodynamics and Molecular Simulation), Higashi-Hiroshima Campus of Hiroshima University, Higashi-Hiroshima, Japan, 25-28 September, **Invited Lecture**
2012-55	Deenesh K. Babi, John M. Woodley, Rafiqul Gani, Jeffrey J. Siirola, Fabrício Rodrigues, 2012, "Process Synthesis, Design and Intensification: An Integrated Approach", AIChE Annual Meeting 2012, Paper 16b, Pittsburgh, PA, USA, 27 Oct - 2 Nov, **CAST Division Plenary Lecture**
2012-56	Amol Hukkerikar, Bent Sarup, Douglas Young, Gürkan Sin, Rafiqul Gani, 2012, "Group Contribution+ (GC+) Based Estimation of Environment-Related Properties for Design of Sustainable Processes: Development of Property Models and Uncertainty Analysis", AIChE Annual Meeting 2012, Paper 137a, Pittsburgh, PA, USA, 27 October to 2 November

2012-57	Igor Mitrofanov, Gürkan Sin, Rafiqul Gani, 2012, "Solventpro: The Solvent Selection and Design Framework", AIChE Annual Meeting 2012, Paper 138a, Pittsburgh, PA, USA, 27 October to 2 November
2012-58	Michele Mattei, Michael Hill, Georgios Kontogeorgis, Rafiqul Gani, 2012, "Design of an Emulsified Hand Wash Through a Systematic Model-Based Methodology", AIChE Annual Meeting 2012, Paper 176c, Pittsburgh, PA, USA, 27 October to 2 November
2012-59	Alberto Quaglia, Alessandra Pennati, Gürkan Sin, Rafiqul Gani, 2012, "A Systematic Approach for Optimized Water Allocation Through Solution of Large Scale Water/Wastewater Networks Problems", AIChE Annual Meeting 2012, Paper 246e, Pittsburgh, PA, USA, 27 October to 2 November
2012-60	Kresten Troelstrup Meisler, Noor Asma Fazli Abdul Samad, Nicolas von Solms, Krist V. Gernaey, Rafiqul Gani, 2012, "Crystallization Kinetics Identification within a Generic Modeling Framework", AIChE Annual Meeting 2012, Paper 300b, Pittsburgh, PA, USA, 27 October to 2 November
2012-61	Deenesh K. Babi, Johannes Holtbruegge, Philip Lutze, AndrzejGórak, John M. Woodley, Rafiqul Gani, 2012, "Process Intensification of the Production of Di-Methyl Carbonate (DMC) Using a New Synthesis and Design Process Intensification Methodology Framework", AIChE Annual Meeting 2012, Paper 304a, Pittsburgh, PA, USA, 27 October to 2 November
2012-62	Emmanuel A. Dada, Azizul Azri Mustaffa, Rafiqul Gani, 2012, "Production of Dialkly Carbonates Via Reactive-Extractive and Pressure-Swing Distillations Using Unifac-CI VLE Model Predictions", AIChE Annual Meeting 2012, Paper 324d, Pittsburgh, PA, USA, 27 October to 2 November
2012-63	Muhammad Zaman, Jay H. Lee, Rafiqul Gani, 2012, "Carbon Dioxide Capture Processes: Sensitivity Analysis for Optimization and Control", AIChE Annual Meeting 2012, Paper 359d, Pittsburgh, PA, USA, 27 October to 2 November
2012-64	Johannes Holtbruegge, Deenesh K. Babi, Philip Lutze, Rafiqul Gani, AndrzejGórak, 2012, "Process Intensification by Membrane-Assisted Reactive Separation Processes: A Design Tool Based On Process Analysis and Optimization", AIChE Annual Meeting 2012, Paper 399a, Pittsburgh, PA, USA, 27 October to 2 November
2012-65	Ravendra Singh, Krist V. Gernaey, Rafiqul Gani, John M. Woodley, 2012, "Adaptive Continuous Template-Based Novel Manufacturing Technique for Faster Manufacturing of New APIs for Clinical Trials", AIChE Annual Meeting 2012, Paper 467e, Pittsburgh, PA, USA, 27 October to 2 November
2012-66	Alberto Quaglia, Bent Sarup, Gürkan Sin, Rafiqul Gani, 2012, "A Systematic Framework for Synthesis and Design of Multi-Scale Processing Networks Using Incremental-Based Solution Strategy", AIChE Annual Meeting 2012, Paper 534c, Pittsburgh, PA, USA, 27 October to 2 November
2012-67	Alberto Quaglia, Bent Sarup, Gürkan Sin, Rafiqul Gani, 2012, "Synthesis and Design of Processing Networks: Decision Making Under Uncertainty", AIChE Annual Meeting 2012, Paper 545a, Pittsburgh, PA, USA, 27 October to 2 November
2012-68	Nor Alafiza Yunus, Krist V. Gernaey, John M. Woodley, Rafiqul Gani, 2012, "An Integrated Methodology for Design of Tailor-Made Blended Products: Biofuels and Bio-Based Lubricants", AIChE Annual Meeting 2012, Paper 546a, Pittsburgh, PA, USA, 27 October to 2 November
2012-69 Poster	Qi Chen, Brianna Christian, Brock C. Roughton, Igor Mitrofanov, Kyle V. Camarda, Rafiqul Gani, 2012, "Simultaneous Design of Ionic Liquids and CO2 Recovery Processes", AIChE Annual Meeting 2012, Paper 599aq, Pittsburgh, PA, USA, 27 October to 2 November

2012-70 Poster	Miguel Mauricio-Iglesias, Gürkan Sin, 2012, "A Model-Based and a Multi-Objective Optimisation Framework for Incremental Scale-Up of Bioreactors", AIChE Annual Meeting 2012, Paper 211g, Pittsburgh, PA, USA, 27 October to 2 November
2012-71 Poster	Fabrício Rodrigues, 2012, "A New Formulation of the Means-Ends Analysis for Process Intensification", AIChE Annual Meeting 2012, Pittsburgh, PA, USA, 27 October to 2 November
2012-72	Thomas Bisgaard, Jakob Kjøbsted Huusom and Jens Abildskov, 2012, "Dynamic Effects of Diabatization in Distillation Columns", 10th European Workshop on Advanced Control and Diagnosis (ACD2012), Lyngby, Denmark, 8-9 November
2012-73	Daniel Olesen, Jakob Kjøbsted Huusom and John Bagterp Jørgensen, 2012, "Optimization based tuning approach for offset free MPC", 10th European Workshop on Advanced Control and Diagnosis (ACD2012), Lyngby, Denmark, 8-9 November
2012-74	Mauricio-Iglesias, M. Valverde-Pérez, B. Sin, G., 2012, "Incremental design of control system of SHARON-Anammox process for autotrophic nitrogen removal", 10th European Workshop on Advanced Control and Diagnosis (ACD2012), Lyngby, Denmark, 8-9 November

	F - Conference Presentations 2013
2013-01	Peam Cheali, 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	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 Poster	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	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	Rafiqul Gani, 2013, "Selection and design of solvents", 23rd Croatian Meeting of Chemists and Chemical Engineers, Osijek, Croatia, 22-24 April, **Plenary Lecture**

2013-10	Amol S. Hukkerikar,Gurkan Sin, Bent Sarup & Rafiqul Gani, 2013, "Molecular structure based property modeling: Development/ improvement of property models through a systematic property-data-model analysis", PPEPPD-2103, Puerto Iguzaú, Argentina, 25-30 May
2013-11	Larissa P. Cunico, Roberta Cerriani, Rafiqul Gani & John P. O'Connell, 2013, "Pure component and phase equilibrium properties prediction in processes involving edible oils and biodiesel production, PPEPPD-2103, Puerto Iguzaú, Argentina, 25-30 May
2013-12	Michele Mattei, Georgios Kontogeorgis, Rafiqul Gani, 2013, "Development of a new comprehensive framework for surfactant selection and design for emulsion based chemical product design", PPEPPD-2103, Puerto Iguzaú, Argentina, 25-30 May
2013-13	Rafiqul 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, **Invited Plenary Lecture**
2013-14	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

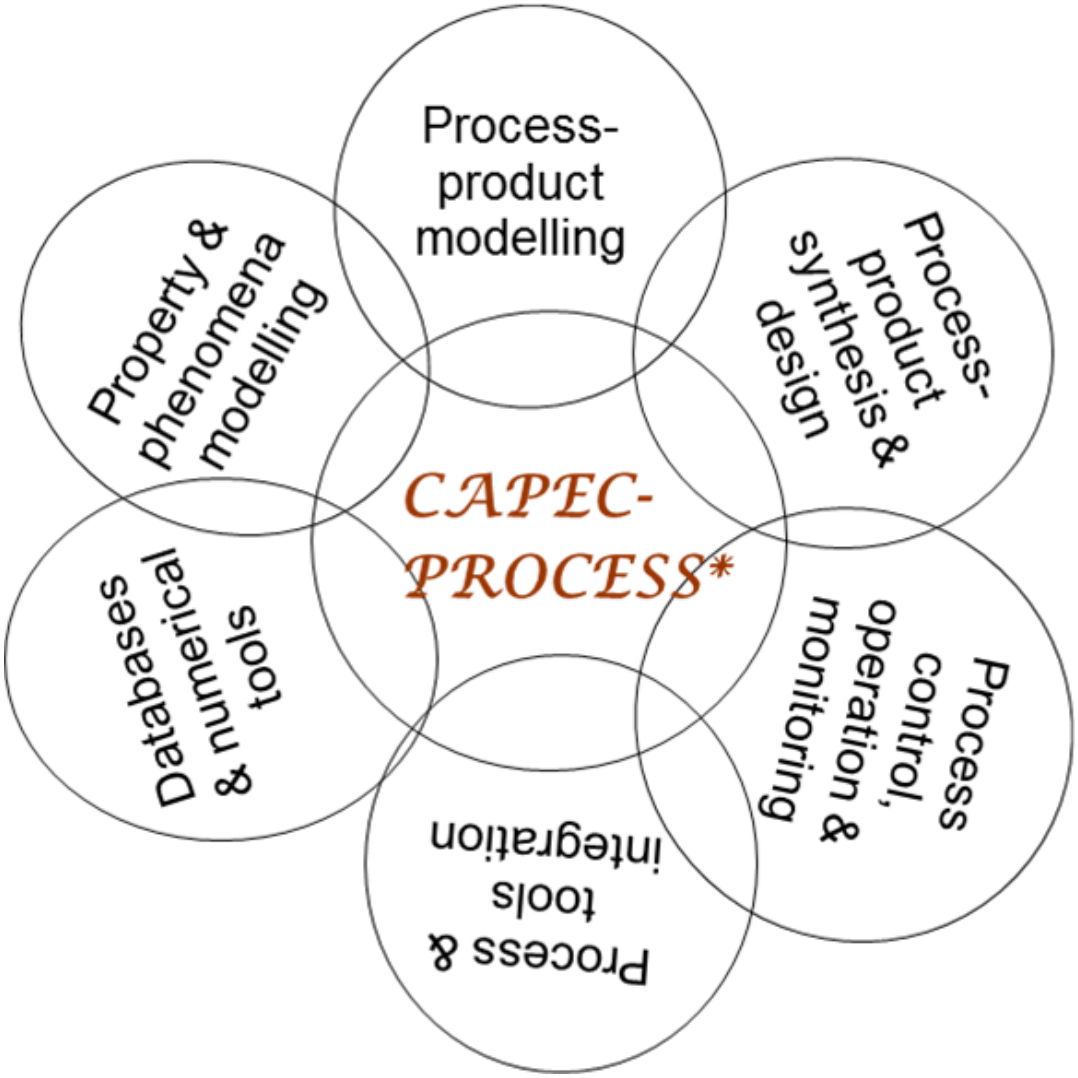
	G – Invited Seminars 2013
	Rafiqul Gani, 2013, "Computer Aided Solvent Selection, Design and Analysis", Bayer Lecture, Carnegie Mellon University, Pittsburgh, PA, USA, 5 March
	Rafiqul Gani, 2013, "Industry-academia collaboration through the CAPEC industrial consortium", Pfizer, Hartford, CT, USA, 7 March

	Upcoming Conference presentations
	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
	Nor Alafiza Yunusa, Krist V. Gernaeya, John M. Woodleya and Rafiqul Gani, 2013, "Design of Sustainable Blended Products using an Integrated Methodology", ESCAPE 23 June 9-12, 2013, Lappeenranta, Finland
	Marina Fedorova, Gurkan Sin, Rafiqul Gani, 2013, "Computer-aided modeling framework – a generic modeling template for catalytic membrane fixed bed reactors", ESCAPE 23, Lappeenranta, Finland, 9-12 June
	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
	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
	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
	Thomas Bisgaard, Jakob Kjøbsted Huusom, Jens Abildskov, 2013, "Dynamic effects of diabatization in distillation columns", ESCAPE 23, Lappeenranta, Finland, 9-12 June

	Remus MihailPrunescu, Jakob Munch Jensen, MogensBlanke 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
	Jing Wu, Laibin Zhang, Morten Lind, Wei Liang, Jinqiu Hu, Sten Bay Jørgensen, Gürkan Sin, Zia UllahKhokhar, 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
	Sawitree Kalakul, PomthongMalakul, KitipatSiemanond, and Rafiqul Gani, 2013, "Software Integration of Life Cycle Assessment and Economic Analysis for Process Evaluation", PSE-Asia, Kuala Lumpur, Malaysia, 23-28 June
	S. Mangnimit, P. Malakul , R. Gani, 2013, Sustainable Process Design of Biofuels: Bioethanol Production from Cassava rhizome",PSE-Asia, Kuala Lumpur, Malaysia, 23-28 June
	Mauricio-Iglesias, Miguel; Sin, Gürkan, 2013, "Accelerating scale-up of bioprocesses using a model-based and multi-objective optimisation methodology", WCCE9 & APCChE2013, Coex, Seoul, South Korea, 18-23 August
	A. K. Vangsgaard, M. Mauricio-Iglesias, K.V. Gernaey and G. Sin, 2013, "Control of a novel energy efficient biological nitrogen removal process", WCCE9 & APCChE2013, Coex, Seoul, South Korea, 18-23 August
	Saranya Mangnimit, PomthongMalakul, and Rafiqul Gani, 2013, "Sustainablbe Process Design of Lignocellulose based Biofuel", WCCE9 & APCChE2013, Coex, Seoul, South Korea, 18-23 August
	Igor Mitrofanov, Gurkan Sin, Rafiqul Gani, 2013, "PSE For Solvent Applications: a Generic Computer-aided Solvent Selection and Design Framework", WCCE9 & APCChE2013, Coex, Seoul, South Korea, 18-23 August
	Sawitree Kalakul, PomthongMalakul, KitipatSiemanond, Rafigul Gani, 2013, "A Generic Life Cycle Assessment Tool For Chemical-biochemical Processes", WCCE9 & APCChE2013, Coex, Seoul, Korea, 18-23 August
	Rafiqul Gani, 2013, "A Process Systems Engineering Approach for Managing the Complexity in Chemical Product-Process Design" WCCE9 & APCChE2013, Coex, Seoul, Korea, 18-23 August, **Invited lecture**
	Rafiqul Gani, 2013, "Industry-academia collaboration through the CAPEC industrial consortium", WCCE9 & APCChE2013, Coex, Seoul, Korea, 18-23 August, **Invited lecture**
	Rafiqul Gani, 2013, "Chemical product design and engineering", XIVe congress of The French Society of Chemical Engineering, Lyon, France, October 8 to 10, **Invited Keynote lecture**
	Mauricio-Iglesias, M. Vangsgaard, A.K. Gernaey, K:G. Sin, G., 2013, "A fuzzy-logic based diagnosis and control of a reactor performing complete autotrophic nitrogen removal", CAB (Computer Applications in Biotechnology), IIT Bombay, India, 16-18 December
	Jason Price, Mathias Nordblad, John M. Woodley, Jakob K. Huusom, 2013, "Application of Uncertainty and SensitivityAnalysisto a KineticModelforEnzymatic Biodiesel Production", CAB (Computer Applications in Biotechnology), IIT Bombay, India, 16-18 December
	Mauricio-Iglesias, M. Montero-Castro, I. Mollerup, A.L. Sin, G., 2013, "Self-optimising control of sewer systems", 10th IFAC International Symposium on Dynamics and Control of Process Systems IIT Bombay, India, 18-20 December
	Thomas Bisgaard, Jakob Kjøbsted Huusom and Jens Abildskov, 2013, "A Modeling Framework for Conventional and Heat Integrated Distillation Columns", 10th IFAC International Symposium on Dynamics and Control of Process Systems, IIT Bombay, India, 18-20 December

7.4 CAPEC-PROCESS Consortium Members

Neste Jacobs Oy



*** Systematic methods and tool**

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