CAPEC-PROCESS Research Report 2011

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CAPEC-PROCESS Industrial Consortium Research Report – 2011

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Preface

This report provides an overview of our research activities and achievements for the period June 2010 to June 2011.

An important new development is the formation of the joint CAPEC-PROCESS industrial consortium. While CAPEC and PROCESS will remain as independent research centers, results from both of the two centers will now be made available to the consortium member companies. In this way, the consortium members will get access to a larger numbers 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, Merlin Alvarado-Morales (PEC10-13), Elisa Conte (PEC10-28), Oscar A Prado-Rubio (PEC10-35), Mohd. Kamaruddin Abdul Hamid (PEC11-02) and Rasmus Wedberg (PEC11-03) have all successfully defended their PhD-theses. At PROCESS, the following co-workers finished their PhD-projects: Daniel Schäpper; Nanna Petersen Rønnest; Muhd. Nazrul Hisham Zainal Alam. At the same time, 7 new PhD-students have started their PhD-projects at CAPEC and PROCESS, while 5 new post-doctoral projects have also been started at the two centers.

Collaborations with our member companies continue to help us to apply our results to interesting industrial problems, to get valuable feedback on our methods & tools and to plan our future projects. Also, collaborations with our friends from academia help us to develop more comprehensive CAPE/PSE models, methods 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, Syngenta, Alfa-Laval, Firmenich and SCG Chemicals from our consortium members, and, Univ of Nancy (France), Chulalongkorn Univ-PPC (Thailand), PROSPECT-UTM (Malaysia), Univ of Kansas (USA) and Auburn Univ (USA) from academia.

We would like to acknowledge the financial support in the form of membership fees from all the consortium members. We would like to thank the Danish funding agencies FTP, EFP and ATV and the EC-research programs under FP-6 and FP-7 for funding of PhD and post-doctoral research projects. Also, we would like to thank the Governments of Malaysia and Mexico for sending students with PhD-scholarships. We would like to welcome Chemtura (NL) and LONZA (CH) as new consortium members.

Finally, we take this opportunity to thank all co-workers of CAPEC and PROCESS for their hard work and dedication. The research results highlighted in this report are their achievements. This is the 14th year since CAPEC as a center and the industrial consortium was established. At CAPEC, Assistant Professor Jakob K Huusom joined as a new faculty member, while Dr. Gurkan Sin got promoted to Associated Professor. At PROCESS, Dr. Ulrich Krühne was promoted to Senior Researcher.

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

Rafiqul Gani & John M. Woodley 1 June 2011

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1. Introduction

1.1 The CAPEC Center

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

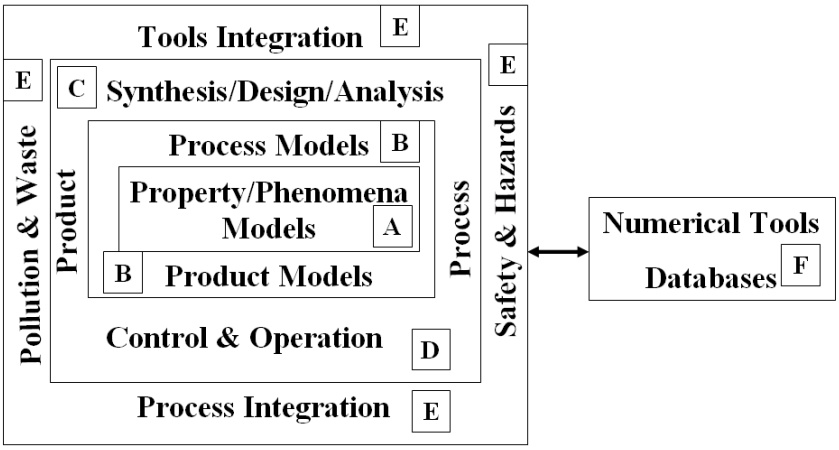


Figure 1.1: Organization of research in CAPEC in terms of research programs

The six research programs are briefly described below:

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

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

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

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

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

Through the industrial consortium, CAPEC co-workers 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.

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.

1.2 The PROCESS Center

The Center for Process Engineering and Technology is focused on the development of new and innovative production processes for industry. PROCESS works at the interface of a number of disciplines, including chemical engineering, biotechnology, process engineering and chemistry. The objective is to provide the necessary infrastructure and support to evaluate and implement the next-generation of processes in the chemical, bio-based and pharmaceutical sectors in particular. All research is carried out in close collaboration with industry and work is carried out at three levels, namely: laboratory-scale experimental process evaluation; model-based evaluation of process technology and pilot-scale 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 6 research area:

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 from batch. New concepts are developed including the creation of a generic process plant.

3. Biocatalytic processes – the development of enzyme (and whole-cell) based processes where high selectivity and mild conditions 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 Technology (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 phramaceutical industry (where the FDA drive such changes).

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

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

- Bio-petrochemicals is a project established in 2007 with the Danish National Advanced Technology Foundation, DTU Chemistry and Novozymes A/S. It is focused on providing a new route to monomer building blocks from sugars such as glucose to enable an alternative route to chemicals from fossil fuels.
- Sustainable Biodiesel is a project established in 2008 with the Danish National Advanced Technology Foundation, DTU Management, Novozymes A/S, Aarhus University and Emmelev A/S. It is focused on developing a new enzymatic route to biodiesel.
- 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, Fermenco ApS 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, ENG-BIO, 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, and is a partner in the F3 European consortium established in 2009. The main focus of F3's activities is the development of early stage pharmaceutical leads in collaboration with AstraZeneca (in UK and Sweden).

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

1.3 CAPEC-PROCESS Activities

While maintaining their unique center activities, it has been decided to join forces on a set of research topics of mutual interest within the pharmaceutical, agrochemical and bio & food industrial sectors. The interaction between the CAPEC and PROCESS centers at the level of the industrial consortium is illustrated through Figure 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.

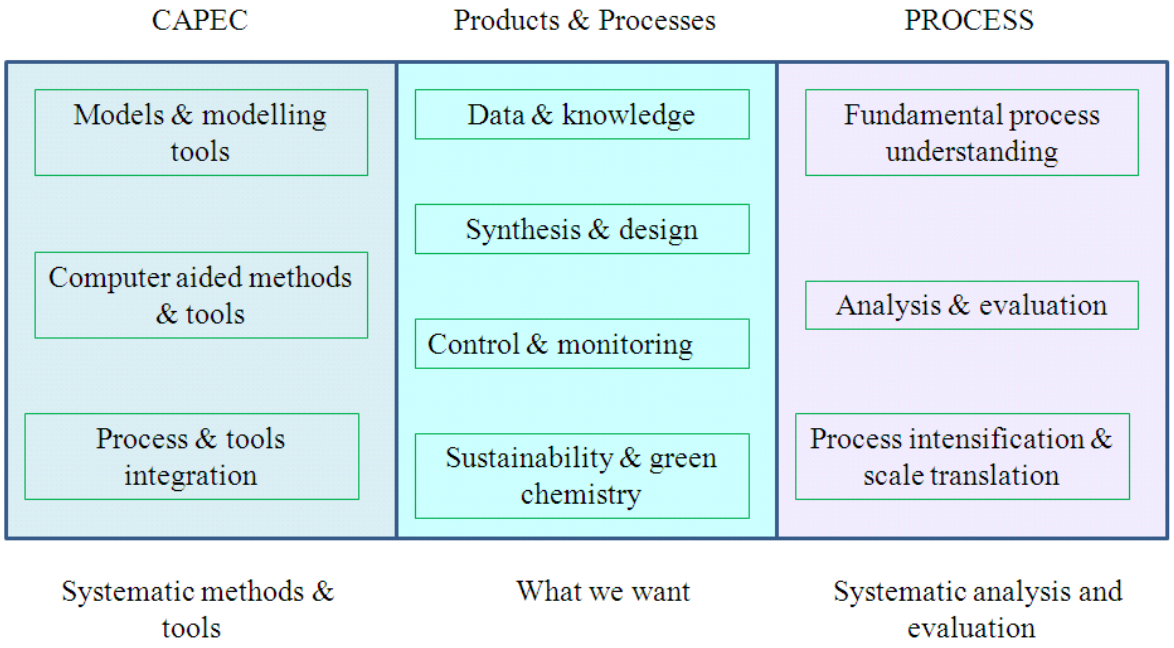


Figure 1.2: Collaboration between CAPEC and PROCESS centers

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.

One of the focus areas of research within PROCESS and CAPEC is process intensification and micro-scale processing. Within this focus area, Associate Professor Krist Gernaey has made good progress in the area of micro-reactors. The figures below illustrate the micro-reactor his research has produced.

Figure 1.3: Assemblying of a micro-reactor

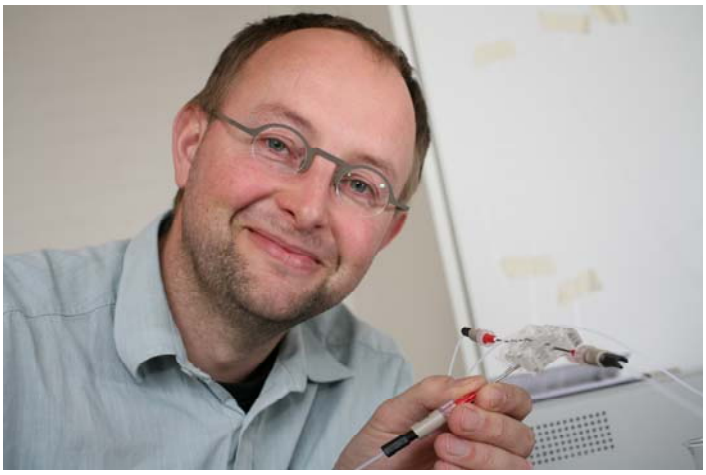


Figure 1.4: Associate Professor Krist Gernaey with an assembled micro-reactor

Table 1.1: Scope and significance of CAPEC-PROCESS research results shown in terms of industries where they can be applied (1: Includes also oil & gas industries; 2: includes also specialty chemicals; * Solving problems in process modelling, simulation, design, analysis and control)

CAPEC Research Programs	Application of Research Results in terms of Industry					
	Petro-chemicals[1]	Chem-icals[2]	Pharma-ceutical	Agro-chemical	Bio & Food	Aroma
Models & modelling tools						
Synthesis, design analysis & evaluation						
Control, operation & Monitoring						
Process & tools Integration						
Databases & Numerical Methods						

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*	Work done during 2010-2011
				More focus given in these areas

Some of the challenges for the future are to use our methods and tools to –

- Find alternative routes for the production of important chemical products in the petrochemical and chemical sectors using renewable resources
- to retrofit or adapt the current processes for changes to bio-based feed materials; to identify new block/platform chemicals,
- to incorporate in all problem solutions the issues related to energy, water, environment and green chemistry.

2. Organization of Activities

2.1 Organizational destails

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

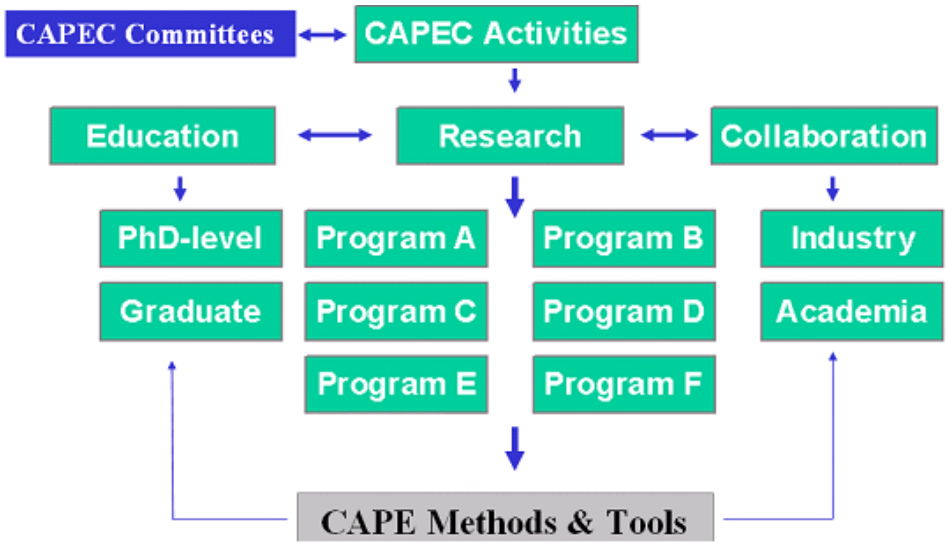


Figure 2.1: Organization of educational and research activities within CAPEC.

The organizational structure of the CAPEC-PROCESS consortium is highlighted through Fig. 2.2, where it can be seen that the consortium now is served by two research centers and has an advisory board consisting of representatives of the member companies and two invited members from academia. Currently 30 companies are members of the consortium.

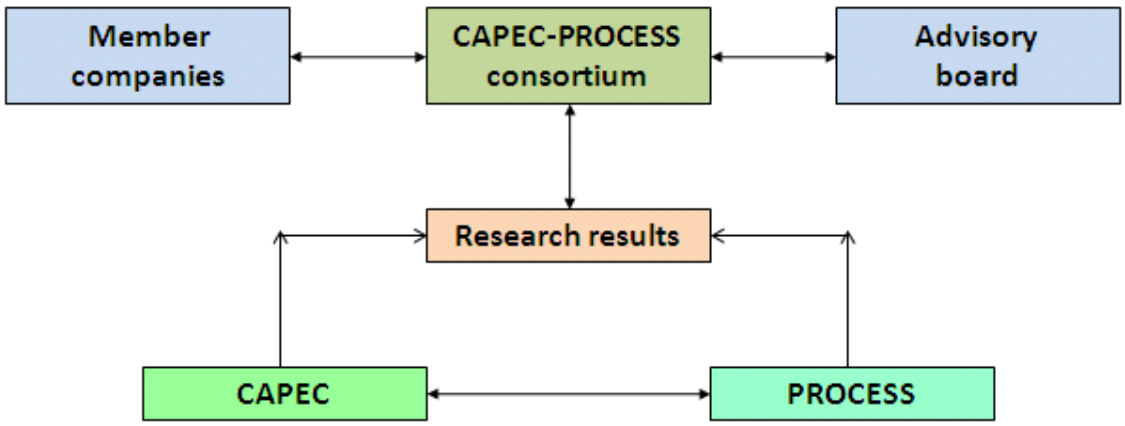
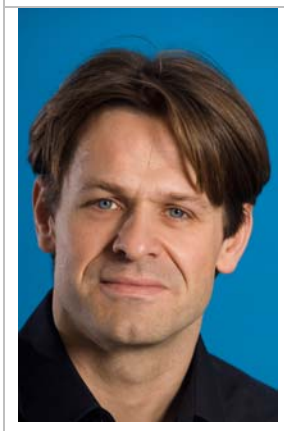


Figure 2.2: Orgnaization structure of the CAPEC-PROCESS consortium

2.2 CAPEC-PROCESS consortium member companies (June 2011)

2.3 Permanent Members

CAPEC	
 **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 Exploration is also being made of process energy requirements, to determine the efficiencies of diabatic distillation processes. Reverse engineering is employed in a set of contexts. Collaborations (outside DK) involve researchers in the U.S., the Netherlands and Germany. ***Research Areas (CAPEC):*** *A, B, F*
 **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*

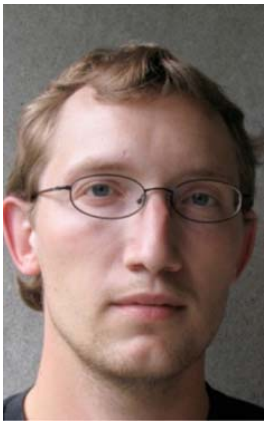
Professor Rafiqul Gani (RaG)

RaG is Director and Co-founder of CAPEC. His research areas of interest covers modelling (properties, process & product); molecular-mixture (product) design; process synthesis, design & analysis; process-tools integration (PAT, sustainable design, intensification, design-control); 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*



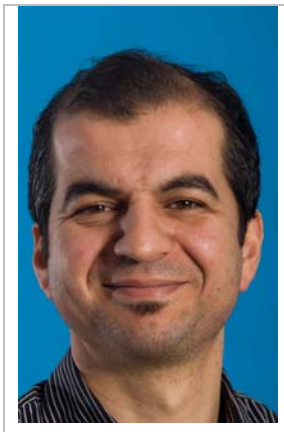
Assistant Professor Jakob K Huusom (JKH)

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 and planned projects are related to applications within: Diabatic distillation; automotive flue gas cleaning; enzymatic production of biodiesel; and polymer production.

Research Areas (CAPEC): *B, D, E*



Associate Professor Gürkan Sin (GSI)

GSI's research covers systematic methods and tools for understanding, design, operation and control of (bio)chemical processes; modeling, control & system identification; uncertainty theory (global uncertainty/sensitivity analysis) & risk assessment; probabilistic-based design paradigm; and, applications in biotechnology, pharmaceutical and water industry. His current research topics of interest are listed below.

- Model-based product - process design; model-based technology configuration, process flowsheet synthesis & process retrofitting
- Product - process design under uncertainty; stochastic programming; risk-based design ; robust decision making under uncertainty
- Dynamics and process control; Integrated process design and control; plantwide control; model-based control and operability analysis
- Uncertainty analysis; Sensitivity analysis; Monte-Carlo simulations
- Process modelling; model identification; model analysis; numerical methods; systems approach
- Process safety and risk assessment

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

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

PROCESS

Associate 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 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

 **Professor John M. 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.
Senior Researchers	
 **Ulrich Krühne (ULKR)**	***Micro process development in chemical engineering*** Microtechnology has gained through the last year's significant importance in chemical engineering. A typical application of microtechnology is the use of plate heat exchangers, using µm scale plate distances, hence improving the heat transfer considerably. Another application field is the production of small amounts of specialised chemicals, where due to lacking economical justification, large scale production facilities are not yet available. The objective of the research activities is therefore the development of microtechnology based processes, which use the advantage of the micro scaled fluid dynamic properties and their influence on chemical, biochemical and physical interactions. A special emphasis is the integration of different unit operations into a single step process, avoiding such the accumulation of inefficiencies of serial performed processes. The starting point of the research will be a FTP project with the title *Novel greener and lean processes using integrated microfactories*. The project aims to demonstrate that fermentation and biocatalysis can be integrated.

Secretary	
 **Eva Mikkelsen (EVA)**	Eva is the administrative secretary for the CAPEC and PROCESS centers and the CAPEC-PROCESS consortium. Eva also serves as the secretary for the editorial office of the Computers and Chemical Engineering journal.
 **Gitte Buggild (GiBu)**	Gitte started on 1 May 2011 as an additional administrative secretary for the CAPEC and PROCESS centers and the CAPEC-PROCESS consortium.

3. Research Projects

3.1 List of current research projects

Research at CAPEC & PROCESS are 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-PROCESS Post Doc	Project Title	Supervisor	Start	End	Funding
Ricardo Morales Rodriquez	Integrated modeling for simulation and design of novel enzymatic processes	GSI/KVG/AM	06-2009	08-2011	FTP
Ravendra Singh	Systematic framework for design and adaption of F3 production processes	RaG/KVG/ JW	09-2009	08-2011	F3 Factory

CAPEC Post Doc	Project Title	Supervisor	Start	End	Funding
Chiara Piccolo	Prediction of phase equilibria involving phase transfer catalysis	RaG	04-2010	03-2012	Syngenta
Elisa Conte	A computer-aided modelling framework for solubility	RaG	09-2010	08-2011	Astra Zeneca
Oscar Andres Prado Rubio	Innovationskonsortiet: Dansk Membran Bioreaktor Teknologi - "MEMBIO"	GJ/JA	06-2010	12-2011	MEMBIO
Miguel Mauricio Iglesias	Analysis of controller performance using dynamic/heat integrated models: An ethanol recovery plant	GSI	10-2010	9-2011	H.C. Ørsted postdoc position
Sascha Sansonetti	The rational selection of lipids for pharmaceutical formulations	RaG	3-2011	2-2012	Astra Zeneca

PROCESS Post Doc	Project Title	Supervisor	Start	End	Funding
Pär Tuvfesson		JW	5-2010		Ambiocas
Mathias Nordblad	Process design and evaluation for enzymatic biodiesel production	JW	12-2008	11-2011	Højteknologifonden (HTF)/Novozymes

Jacob Skibsted Jensen	Biopetrochemicals	JW		10-2011	Novozymes
Nanna Rønnest Petersen	Population heterogeneity in fermentors	KVG			FøSu
Ulrika Türnvall	Development of the next generation biocatalysts for industrial production of chemicals	JW	1-2011	1-2013	Ambiocas/Bionexgen

CAPEC-PROCESS PhD Student	**Project Title**	**Supervisor**	**Start**	**End**	**Funding**
Albert Emili Cervera Padrell	Moving from batch towards continuous organic-chemical pharmaceutical production	KVG/SK/ RaG	8-2008	7-2011	DTU
Philip Lutze	Development of a systematic synthesis methodology for achieving process intensification	JW/RaG/	12-2008	11-2011	DTU
Alicia Román-Martinez	Design of intensified bioprocesses	RaG/JW	7-2008	6-2011	PROMEP, Mexico
Wenjing Fu	Process Design of Chemo-enzymatic Synthetic Cascades	JW/RaG	3-2008	5-2011	DTU
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	12-2011	Malaysia
Naweed Al-Haque	Modelling controlled release of substrate and removal of product in biocatalysis	JW/PT/RaG	11-2009	10-1012	DTU/AMBIOCAS
Anna Katrine Vangsgaard	Modeling and Control of Novel Membrane Processes for Autotrophic Nitrogen Removal	KVG/GSI/ 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

CAPEC PhD Student	**Project Title**	**Supervisor**	**Start**	**End**	**Funding**
Martin Dela Ellegaard	Thermodynamic properties and phase equilibria from fluctuation solution theory	JA	2-2008	1-2011	DTU
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	12-2011	Malaysia
Carlos Axel Díaz Tovar	Computer modelling of lipid processing technology	RaG/Bent Sarup	3-2008	7-2011	DTU/Alfa Laval
Martina Heitzig	Computer-aided modelling for efficient and innovative product-process engineering	RaG/GSI/ PGL	12-2008	11-2011	DTU
Azizul Azri Bin Mustaffa	Development and analysis of Group-	RaG/GK	4-2009	3-2012	Malaysia

	Contribution^{plus} models for property prediction of organic chemical systems				
Nor Alafiza Yunus	Tailor-made design of chemical products: Bio-fuels and other blended products	RaG/JW/ KVG	7-2010	7-2013	Malaysia
Amol Hukkerikar	Model based integrated process-product design – retrofitting and optimisation	GSI/RaG BS	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	10-2013	MultiMod

PROCESS PhD Student	Project Title	Supervisor	Start	End	Funding
Linfeng Yuan	Membrane Assisted Enzyme Fractionation	GJ/JW	3-2008	2-2011	Novozymes
Bodil Voss	Value-added chemicals from biomass by Heterogeneous Catalysis	JW/NCS/JDG	5-2008	4-2011	Industrial PhD Haldor Topsøe
Paloma de Gracia Andrade Santacoloma	Multi-enzyme process modelling	JW/KVG/GSI	11-2008	10-2011	DTU
Yuan Xu	Evaluation of new process technology for lipase-catalyzed biodiesel production	JW/MAN/LGK	3-2009	2-2012	HTF (højteknologifonden)
Mads Orla Albæk	Investigation of the efficiency of alternative enzyme production technologies	KVG/SMS/ MSH	4-2009	3-2012	Industrial PhD Novozymes/VTU
Rita Lencastre Fernandes	Population balance models and computational fluid dynamics: a model framework to describe heterogeneity in fermentors	KVG/AJ/IN	11-2009	10-2012	DTU/KT FøSu
Joana de Lima Ramos	Guiding biocatalytic process improvements using engineering evaluation tools	JW/PT	3-2010	2-2013	Biotrains (Marie Curie ITN, Grant agreement no.: 238531)
Andrijana Bolic	Monitoring Continuous Fermentation Processes in Mcirobioreactor Systems	KVG/AEL/KR/ NX	3-2010	2-2013	FøSu
Watson Lima Afonso Neto	Integrated downstream processing for biocatalytic reactions	JW/PT	6-2010	5-2013	Biotrains (Marie Curie ITN, Grant agreement no.: 238531)
Aleksandar Mitic	Operational aspects of continuous pharmaceutical production	KVG/KDJ	11-2010	11-2013	DTU/Lundbeck/MP2T
Kresimir Janes	Scale-up of biocatalytic cascade reaction for the	KVG/PT	12-2010	11-2013	Ambiocas

	synthesis of chiral amines				
Rui Xue	Reactor and Process Design for Multi-enzymatic Synthesis	JW/AM/JDM	12-2010	11-2013	HMO project
Vijaya Krishna Bodla	Integrated Microfactories for enzyme production	KVG/JW	3-2011	2-2014	FTP

External PhD-Students	**Project Title**	**Supervisor**	**Start**	**End**	**Funding**
Susilpa Bommareddy	A framework for computer aided process flowsheet design	MRE/RaG	4-2010	7-2010	Auburn Univ (US)/CAPEC
Klaus Reinholdt Nyhuus Hansen	New Product Introduction for the Pharmaceutical Industry	MG/RaG	9-2009	8-2012	DTU Management
Lida Simasatitkul	Design of Reactive Distillation for Biodiesel Production from Free Fatty Acid	AA/RaG	3-2011	2013	Chulalongkorn University (Thailand)
MSc-project Students	**Project Title**	**Supervisor**	**Start**	**End**	**Funding**
Preeyaporn Saengwirun	Development of economic analysis methods and tools for process design	RaG	5-2010	9-2010	PPC,Thailand /CAPEC
Jeerawat Wannaborworn	Solvent-based separation	RaG	5-2010	9-2010	PPC,Thailand /CAPEC
Mehboob Nawaz	Optimal biorefinery	RaG/Edwin Zonderwan	6-2010	12-2010	ERASMUS
Naruporn Narot	Sustainable process design study of cellulosic-based biofuels	RaG	5-2010	9-2010	PPC, Thailand/ CAPEC
Ankit Khandelwal	Solvent based organic synthesis	RaG	9-2010	8-2011	40 points/Cheminova
Pierre Godfrey	Design of Sustainable Separation Processes	RaG	1-2011	6-2011	30 points
Siliva Melendez Prat	Evaluation of Immobilization Supports for Enzymatic Biodiesel Production	JA	2-2011	6-2011	20 points
Rasmus Enemark-Rasmussen	A framework for computer-aided (HAZOP) studies supported by dynamic simulations	GSI	1-2011	6-2011	Kongsberg/Mærsk Olie & Gas
Guillermo Serrano Briega	Evaluation of coupled dehydrogenase systems	JW/PSA	12-2010	6-2011	30 points
Hemalata Ramesh	Continuous production of alkyl esters	JW/MAN	02-2011	07-2011	30 points
Rolf Ringberg	Chemoenzymatic combination of TS-1 and GO-x	JW	2-2011	6-2011	30 points/Haldor Topsøe/Novozymes

3.2 CAPEC-PROCESS research programs versus co-workers

Table 3.2a provides an overview of the research programs and the CAPEC personnel involved with them

Research Programs	**CAPEC coworkers & research activities**				
	Faculty[1]	**Post-Docs**[2]	**PhD-students**[3]	**MSc-students**[4]	**Others**[5]
A: Property & Phenomena Modelling	**JA**; RaG	ChP; ELC; SSA	ADI; AZM; *NOY*, AMH; *(RAW; MEC);* Mattei	SM Prat; (*M Mettei*)	*B C Roughton*
B: Product & Process Modelling	**RaG**; GSI; JA; JKH	RMR; ChP; MMI; RS	ADI; *NAS*; *ARM*; MAT; *WF*; AMH; AQ; *NAH*; *AKV; KreTM; (OAP); Babi*	A Khandelwal; (*P Saengwirun*)	L Simasatitkul*;* (*S Sansonetti*)
C: Synthesis, Design & Analysis	**GSI**; RaG	*RS*, ELC, MMI; SSA	ADI; *ARM*; AZM; *ACP*; *PIL*; *WF*; *NOY* ; IGM, *KreTM; (MKA; ELC);* Mattei	A Khandelwal; P. Godroy; (*J Wannaborworn*)	*S Bommareddy*; *B C Roughton*; L Simasatitkul; *A Janthasurak*
D: Control, Operation & Monitoring	**JKH**; GSI; RaG; (KHC)		*NAS*; (*MKA; OAP*); *NN*	R Enemark-Rasmussen	
E: Process & Tools Integration	**GSI**; RaG; JKH	*RS*	MAT; *PIL*; AMH; AQ; *KreTM*; IGM; *AKV*; KRNH; *(MAL; MKA); Babi*	P. Nidhinandan; (*N Narot; M Newaz*)	
F: Databases & Numerical Methods	**JA**; RaG				
Currently active	**4**	**5 + 1**	**8 +8 + 3**	**4**	**1+3**

1: Research area coordinators are indicated in bold; 2: Post-docs shared with PROCESS are indicated in italic; 3: PhD-students who are shared with PROCESS are indicated in italic; PhD-students who have finished are indicated in italic-parenthesis; 4: MSc-students who have finished are indicated in italic-parenthesis; 5: External (or visiting) PhD-students who have returned to their home university and finished their PhD are indicated in italic-parenthesis; those who have returned but are still continuing as PhD-student are indicated in italic. All other names indicate current coworkers at CAPEC.

Table 3.2b provides an overview of the research programs and the PROCESS personnel involved with them

Research Programs	**PROCESS coworkers & research activities**				
	Faculty[1]	**Post-Docs**[2]	**PhD-students**[2]	**MSc-students**	**Others**
1: Micro reactors	**KVG**; JW; ULKR*		VKB; AB		
2: Continuous processes	KVG; **JW**	JSK; *RS*; MAN	*ACP*; YX; AM	R Ringberg	
3: Biocatalytic processes	KVG; **JW**	UT; PT; MAN	*WF*; PAS; YX; *NAH*; JLR; WAN	GS Briega; H Ramesh	B Mxynorozyk; S Thomsen, M Vestphael; AT Pedersen
4: Process intensification & intensified unit operations	KVG; **JW**	*RS*	*PIL*; LY; BV, MOA; NAH; RLF; *ARM; NOY; AKV*		
5: PAT	**KVG**; JW		*NAS*, *KreTM*		
6: Scale translation	KVG; **JW**	PT; MAN	KJ; RX		
Currently active	**2 + 1**	**4 + 1**	**13 + 8**	**3**	**4**

1: Research area coordinators are indicated in bold; * indicates Senior Researcher; 2: Post-docs shared with CAPEC are indicated in italic; 3: PhD-students shared with CAPEC are indicated in italic; All other names indicate current coworkers at PROCESS.

3.3 Post-Doctoral Research Project Overview

Elisa Conte (ELC) 	***A framework for API solubility modelling*** The solubility of solid organic compounds in water and organic solvents is a fundamental thermodynamic property for many purposes such as product-process design and optimization for the chemical and pharmaceutical industries. This work aims at developing an efficient framework for the solubility modelling of Active Pharmaceutical Ingredients (API). With this framework, the user will be able to solve a specific design/verification problem, quickly and simply with little expert knowledge. A solubility database containing solid-liquid equilibrium data is at first developed. Then, available and validated models for the calculation of solid-liquid equilibrium are used for solubility calculations when the needed model interaction parameters or experimental data are available (the UNIFAC-CI method is used when the GC-models lack interaction parameters). A new GC^{+} model for APIs solvent selection based on the hydrophobicity, hydrophilicity and polarity information of the API and solvent is also developed for performing fast solvent selection and screening. Eventually, all previous developments will be integrated in a computer-aided framework for their efficient and integrated use. *Research areas: A, F – Property/phenomena models; Databases*
Miguel Mauricio Iglesias (MMI) 	***Modeling and control of heat-integrated distillation columns: An industrial case study*** Strategies for heat recovery in distillation processes have been extensively implemented in industrial processes during the last decades. However, operation and control of heat-integrated systems becomes a formidable challenge if not a problem since different time-scale phenomena interact. This project has two aims; firstly to create a systematic framework for the modeler for developing dynamic models of distillation process with heat-integration. To this end a computer-aided methodology is developed. Secondly, the methodology is tested in an actual industrial case, where the aforementioned model is used to analyze and solve operation and control problems. Two solutions will be presented for improving its control: i) a fine tuning of the existing control strategy, therefore suitable for immediate implementation; and ii) a new control structure, including sensors and actuators for long term modification of the system. The suitability of the proposed control strategies will be ultimately evaluated using as input actual data of one month of operation. *Research area: B, D - Process Modelling, Simulation and Identification*

Mathias Nordblad (MAN) 	***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*
Chiara Piccolo (ChP) 	***Prediction of phase equilibria involving phase transfer catalysis*** Phase transfer catalysis (PTC) has the potential to stand out as an attractive alternative to conventional processes for the synthesize of special organic chemicals, from two immiscible reactants, that normally will not contact each other: in PTC systems a phase transfer catalyst acts as a shuttle between a polar phase that contains the salt reactants and a non-polar phase that contains the organic reactants. Many factors affect PTC processes, for example, choice of the organic phase, choice of the catalyst, presence of extra ionic species, temperature, stirring rate. The aim of this project is to enable semi-quantitative and quantitative estimations of phase equilibria involving PTC and, ultimately, to develop a systematic methodology to select the best system features and operating conditions for a given synthesis. This screening strategy should take into account the knowledge gained from data and model-based analysis of solubility and phase equilibria of the reacting systems. *Research area: A; B; C* *Property modelling; process modelling and analysis*

Oscar Andres Prado-Rubio (OAP)

Dynamic membrane bioreactors (MBR) technologies for waste water treatment

In the last couple of years, membrane bioreactor technologies have attracted attention for waste water treatment. The reasons are a notably better effluent quality, operation at higher cell densities and significantly reduction in the plant size. Relevant challenges operating MBR are the membrane fouling and concentration polarization effect, which are influenced by inflow/ membrane/module characteristics and operating conditions. Interactions between those parameters are not fully understood.

The aim of the project is to investigate operational fouling/concentration polarization control though dynamic membrane devises, which can potentially be employed in waste water treatment plants. A vibrating hollow fiber module and high frequency back flushing system are under investigation. The purpose is to evaluate their potential to reduce the adverse influence of membrane fouling and concentration polarization that could be associated to biological treatment of waste water. Therefore, through system understanding, operational ways to minimize their adverse influence could be proposed.

Research area: C, D, E
Synthesis, design and analysis; Control and operation; Pollution and waste.

Sascha Sansonetti (SSA)

The rational selection of lipids for pharmaceutical formulation

Lipidic dose forms are applicable to both the early and late stages of product development in the pharmaceutical industry. They are most frequently used to formulate Active Pharmaceutical Ingredients (API's) with inherently poor aqueous solubility. They can also be used to avoid a solid dose form and the solid state issues that often blight this category.

The aim of the project is to develop a software tool to predict the thermodynamic solubility of drug molecules in high molecular weight liquids.

Research area: A, C
Property mdelling, formulation design, software development

Ravendra Singh (RS)

Systematic framework for design and adaption of "Flexible, Fast, and Future - F^3" production processes

The objective of this project is to develop a systematic framework and a generic "Substrates Adoption" methodology through which a fast and flexible continuous modular plant (F^3 plant) can be designed and adapted for a series of similar substrates or changes in the F^3 plant. The changes can be related to process operational conditions as well as in the physical arrangement of the process equipments. The supporting tools for the substrates adoption are:

- a knowledge base consisting of the properties of substances (reactants, products, reagents, solvents, and catalysts), reaction characteristics and characteristics of unit operations;
- a model library consisting of the thermodynamic models and process operational models.

The systematic framework, the methodology and the supporting tools have been developed and their scope and significance have been demonstrated through a conceptual example.

Research Area. A, B, E
Continuos-Batch process design & analysis

Ricardo Morales-Rodriguez (RMR)

Integrated modelling for simulation and design of novel enzymatic processes

The project aims at understanding the dynamic simulation of enzymatic processes (such as, bioethanol production) for better design and technological evaluation purposes. Therefore, a Dynamic Lignocellulosic Bioethanol (DLB1.0) modeling platform was developed to investigate the interaction among the different units having different operating strategies (such as, fed-batch, continuous and continuous-recycle). This project has also involved the development of a mathematical model for the Simultaneous Saccharification and Co-Fermentation unit (SSCF). The validation of inhibition effects on enzymatic hydrolysis in another of the milestones reached in this project, which ensures the reliability of the model for plant design purposes. Uncertainty and sensitivity analysis has been also performed on the DLB1.0 as a previous step for stochastic optimization (using Monte-Carlo technique) for further model analysis and optimal process operation. Finally, it is expected that the obtained results will identify new avenues for improved biofuels processing strategies using lignocellulosic feedstock, as well as being useful for providing operator training in the plant.

Research area: B, C, D, E

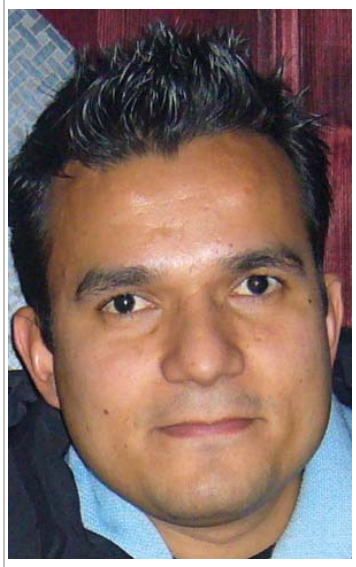
Pär Tufvesson (PT) 	***Biocatalytic production of chiral amines using transaminases*** Project Description: Biocatalytic transamination is being established as key tool for the production of chiral amine pharmaceuticals and precursors due to its excellent enantioselectivity as well as green credentials. Recent examples demonstrate the potential for developing economically competitive processes using a combination of modern biotechnological tools for improving the biocatalyst alongside using process engineering and integrated separation techniques for improving productivities. However, many challenges remain in order for the technology to be more widely applicable, such as technologies for obtaining high yields and productivities when the equilibrium of the desired reaction is unfavorable. The current project adresses these process challenges and develop strategies to overcome them, and aim to understand these and their applicability based on fundamental principles. *Research area: Process evaluation, Biocatalysis*
Ulrika Törnvall (ulrt) 	***Development of the next generation biocatalysts for industrial production of chemicals*** A major hurdle for a widespread implementation of biocatalysis in industry is the lack of appropriate process technology, especially in fields where extra demands are placed on the process, such as oxidation reactions. In this project, oxidation reactions catalyzed by oxidases and/or Baeyer-Villiger monooxygenases will be used as model reactions to develop a standardized methodology, a “process discovery platform”, which will guide researchers in the establishment of cost-efficient and environmentally friendly industrial bioprocesses. In the first instance, scale-down laboratory reactors and processes will be used to assess new configurations and modes of operation. In the latter stages of the project, pilot-plant trials will serve as an assessment and a demonstration of the new process technology on selected targets. After collection of kinetic, stability and thermodynamic data, these will be used for process modelling from a technical and economic perspective. In order to evaluate also the environmental benefits, simplified life cycle assessments of the developed technologies will be performed. *Collaborators: University College London, Slovak University of Technology, CLEA Technologies B.V., LentiKat´s a.s.*

3.4 PhD-Research Project Overview

Naweed Al-Haque (NAH)  PROCESS-CAPEC	***Modelling of controlled substrate supply using solid sorbents in biocatalysis*** With the development of biocatalysts, greener technologies have become more accessible to industry. Biocatalysis has become increasingly common in all industrial sectors such as chemicals, fuels, food and pharmaceuticals. The obvious advantage of this technology is selectivity which is necessary to obtain a high yield of a specific product. The other advantages of operating in benign operating conditions make it an alternative worth investigating. However In bioprocesses, especially in bioconversions, the substrate and the product may inhibit or damage the biological catalyst or interfere with other components in the reaction medium above a critical concentration. This limitation can be overcome with methods such as *in-situ* product removal (ISPR) and *in-situ* substrate supply (ISSS) using solid sorbents. This project will focus on the latter issue and in particular for the development of this novel substrate release technique with controlled diffusing rate of the substrate in the reaction medium using a solid resin(s). *Research area: Biocatalysis, controlled substrate supply, resins, ISPR, mathematical modelling*
Mads Orla Albæk (MAOA)  PROCESS	***Investigation of the efficiency of alternative enzyme production technologies*** Low enzyme costs are essential for establishing a sustainable production of 2nd generation cellulosic ethanol. The aim of the thesis is to objectively compare alternative enzyme production technologies with the current industrial practice. The project strategy is to construct a process model based on a relevant production organism and use the model in screening the open literature for alternative technologies. The model consists of a reactor model describing the mass transfer characteristics of the system and a biological model of the production organism. The biological model includes maintenance uptake of substrate and oxygen as well as rheological development throughout the fermentation process. This is an industrial PhD-project that is carried out at Novozymes A/S. *Research area: Enzyme technology; Reaction and transport engineering*

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 analysed. *Research area: Microreactors; Biocatalysis*
Andrijana Bolic (ANB)  PROCESS	***Monitoring continuous fermentation processes in microbioreactor systems*** The objectives of this project are to perform continuous cultivations with *Saccharomyces cerevisiae* in a microbioreactor, and to implement NIR and Raman spectroscopy for rapid on-line measurement of process variables like substrate and biomass concentration. In order to obtain a vast amount of reliable experimental data, it is important to perform continuous cultivations in a reproducible manner with good control of process parameters (T, pH, DO and OD). Thus one part of the project will be devoted to assessment and improvement of the existing microbioreactor platform at DTU-KT. The microbioreactor performance will be thoroughly evaluated and benchmarked against continuous culture yeast cultivations in lab-scale reactors. Afterwards, NIR and Raman spectroscopy will be added on to the system, and the capability of both methods to measure cultivation process variables will be evaluated based on experimental data and chemometric models. The obtained spectra will also be analyzed with the aim to observe changes in the properties of the microorganism population (heterogeneity of cells). External supervisors: Anna Eliasson Lantz (DTU Systems Biology), Nicolas Szita (UCL, London, UK), Karsten Rottwitt (DTU Fotonik) *Research area: Microbioreactors, On-line monitoring, Fermentation*

Carlos Axel Diaz-Tovar (ADI)



CAPEC

Computer aided modeling of lipid processing technology

The production of edible fats and oils, like many other chemical processes, involves a wide range of processing steps, from crude edible oil (vegetable) extraction to the final product. However, unlike the chemical processes, the state of the art in process modeling and simulation has only to a very limited extent penetrated this industry, and part of the reason is the complex nature of the lipid systems involved. Modeling and validation of physical properties for the most representative chemical species (and their mixtures) occurring in the edible oil industry, as well as optimization of the associated unit operations and process sections are the main objectives of this PhD project.

A large lipid database has been developed. A collection of models for pure component properties of lipids has been developed and validated. Using these property models, edible oil production processes have been simulated and analyzed.

This project is partially funded by Alfa Laval.

Research area: A, B, C, F
Property-Process modeling; Process design; Database

Rita Lencastre Fernandes (RLF)

PROCESS

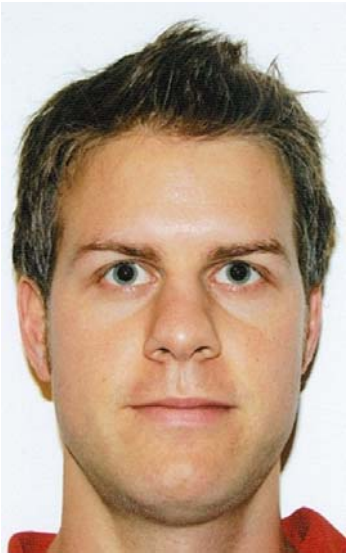
Population balance models and computational fluid dynamics: a model framework to describe heterogeneity in fermentors

The project focuses on the development of models that can predict the growth and behaviour of heterogeneous microbial populations. Experimental data is used to formulate Matlab based models that can predict changes in the microbial distributed properties (e.g. single cell protein content, growth and productivity) due to varying environmental conditions in the fermentor. In a later stage, the population model will be integrated with a fluid dynamics model for a stirred reactor, allowing for predicting process behavior under different environmental conditions. The project is partly funded by the Danish Council for Strategic Research in the frame of the project "Towards robust fermentation processes by targeting population heterogeneity at microscale", and developed in tight collaboration with the ERA-NET Industry Biotechnology project "Targeting population heterogeneity at microscale for robust fermentation processes".

Research area: Process-product modelling/design

Wenjing Fu (WFu)  PROCESS - CAPEC	***Process design of chemo-enzymatic synthetic cascades*** Limited fossil resources and the unstable oil price make it increasingly important to create new chemical processes based on renewable resources. For many of these new processes a combination of enzymatic as well as heterogeneous and homogeneous catalysis will be required to direct the reaction toward the desired products. In many chemo-enzymatic synthesis processes, even a small reaction pathway, there are many alternative technologies. Thus, there is a need for a systematic methodology capable of evaluating different processes in order to identify the optimal set of products and the best route for producing them. In particular this PhD project will focus on the design of chemo-enzymatic synthetic cascades from glucose to 2,5-furandicarboxylic acid (FDA) as a case study. The process will form the basis of process / cost models for sensitivity analysis and to set targets for catalyst and process improvements. *Research area: Process design; Chemo-enzyme synthesis; process evaluation*
Martina Heitzig (MAT)  CAPEC	***Computer-aided modelling for efficient and innovative product-process engineering*** Computer-aided modelling plays a role of increasing importance through a number of industries related to chemical and biochemical engineering due to its ability to reduce the number of cost-intensive, time-consuming and resource-demanding experiments but also because it has the potential to deliver truly innovative solutions that might not necessarily be obtained by conventional trial-and-error approaches. The core perquisite however, is to provide predictive models that are able to represent the investigated systems to the degree of detail required for the special application. The objective of this project is to systematize the process of model development and increase its efficiency by developing a computer-aided modelling framework that provides the required work- and data-flows to solve a large variety of different modelling problems. The framework guides the user through the work-flow, combines the required tools and database connections where needed and offers expertise the user might not have. The framework supports multi-scale modelling and the archiving and re-use of models. *Research area: B, E* *Computer-aided modelling; modelling framework; multiscale; multidimension; ICAS-MoT*

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 optimisation 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. *Research area: A, B, C, E* *Process modeling, simulation and identification; Process-product synthesis, design and analysis; Process and tools integration.*
Krešimir Janeš (kreja)  PROCESS	***Scale-up of biocatalytic cascade reactions: transaminase catalysed synthesis of chiral amines*** New small molecule pharmaceuticals are preferably produced as single enantiomers due to safety and regulatory concerns. *Biocatalysis* is a very good option for this production and is already established in industry owing to its green profile and superior stereoselectivity. One challenge that needs to be met in this type of process is to overcome the disadvantageous thermodynamic equilibrium for the reaction. This can be done by degrading or recycling one of the reaction co-products *in-situ* using additional enzymatic reactions. These cascade systems have been shown to be feasible in micro-litre scale, however the systems need to be characterized and be shown to be scalable and economically feasible to be able to be industrially implemented. In this project different multiple enzyme cascade systems coupled to transaminase synthesis of chiral amines will be evaluated and characterized using scaled down test models. Design and selection of one or more process set ups for scale up experiments will be performed and the scale effects will be determined. *Research area: Biocatalysis; Chiral synthesis; Transaminase*

Philip Lutze (PIL)  PROCESS-CAPEC	***Development of a systematic synthesis/ design methodology incorporating process intensification*** Process intensification (PI) has the potential to improve existing processes or create new process options, which are needed in order to produce products using more sustainable methods. In principle, an enormous number of intensified process options can be generated but where and how the process should be intensified for the biggest improvement is difficult to identify. Therefore, the objective of this work is the development of a systematic computer aided synthesis and design methodology incorporating PI. To manage the complexities involved, the methodology employs a decomposition based solution approach. Starting from an analysis of existing processes, the methodology generates a set of process options and reduces their number through several screening steps until from the remaining options, the optimal is found. The developed methodology together with its associated tools and algorithms will be tested and verified with case studies from the chemical, biochemical and pharmaceutical sectors. *Research area: C, E* *Synthesis/design & analysis; Process and tools integration*
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. *Research area: B, C, D* *Crystallization; Crystal size distributions; Process modelling, simulation and identification; Process monitoring and analysis*

Aleksandar Mitic (ASMI)  PROCESS	***Operational aspects of continuous pharmaceutical production*** Organic synthesis is essential for production of an important class of pharmaceuticals. To date, pharmaceutical production is mainly based on batch and semi-batch processes and involves 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. For those purposes, the potential use of micro-scale equipment, such as microreactors and L-L microseparators will be tested. Furthermore, in the second phase of this PhD project the main focus will be on on-line monitoring and control of the established continuous process. Applications of NIR spectroscopy will be tested. *Research area: continuous pharmaceutical production, process analytical technologies, 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. *Research area: C, E, F* *Computer Aided Molecular Design; Solvent selection; ICAS*

Azizul Azri Mustafa (AZM)  CAPEC	***Development and analysis of GC^{Plus} models for property prediction of organic chemical Systems*** Accurate, reliable and efficient prediction of properties is very important in chemical process-product design. However, due to the increased complexity of the molecular structures of chemicals, their wider applications, and demands for greater accuracy, extension and analysis of the current prediction methods as well as development of new models are necessary. Therefore, the combination of group-contribution (GC) and atom connectivity (CI) (the GC^{Plus} approach) that is able to extend the application range of the host property model has been developed and extended to predict the UNIFAC GC-model parameters (see PEC09-17). The objectives of this PhD-project is to analyze the performance of the GC^{Plus} approach in VLE and SLE calculations and based on it, to extend and further develop the GC^{Plus} approach for other versions of the UNIFAC models and to apply the models for chemical process synthesis and design. *Research area: A, B, C* *GC^{Plus} approach; mixture properties; UNIFAC models; parameter prediction*
Alicia Román Martínez (ARM)  CAPEC-PROCESS	***A model-based framework for design of intensified enzyme-based processes*** The objective of this project is to develop and apply a flexible framework for design and analysis of intensified enzyme-based processes. The framework consists of a systematic model-based computer aided methodology to identify reliable, feasible and/or improved intensified design options for enzyme-based processes. The framework incorporates tools for process synthesis and optimization, such as, the use of superstructures and strategies for development of mathematical models to find the best route for the synthesis of specified products through enzyme-based process. The advantages of using this framework is that it permits the saving of valuable experimental resources, which could then be used only for implementation and verification of the design and is able to enumerate and analyze all the possible reaction-separation schemes in the process to locate a reduced search space where the best option could be found. Current work is developing case studies in the pharmaceutical and renewable fuels area to highlight the application of the framework. *Research area: C; E* *Process technology and unit operations; Process synthesis*

Watson Neto (WAN)  PROCESS	***Downstream processing for biocatalytic reactions*** Chiral amines are important building blocks for pharmaceutical and chemical industries and they can be produced enzymatically with high enatioselectivity using ω-transaminase (EC 2.6.1.18). However, the use of this enzyme has some drawbacks such as substrate and product inhibition and unfavorable equilibrium which together limit the process productivity. In order to make its industrial utilization more attractive and efficient, these drawbacks need to be evaluated and addressed. The aim of this project is to characterize this process and develop technology for an efficient integrated downstream process (*in situ* product removal - ISPR) for chiral amines that allow both alleviating these drawbacks hence increase the productivity, thereby increase the process attractiveness. *Collaborations: Lund University (BIOTRAINS Network) c-Lecta GmbH*
Albert Emili Cervera Padrell (ACP)  PROCESS-CAPEC	***Moving from batch towards continuous organic-chemical pharmaceutical production*** Organic synthesis based pharmaceuticals have traditionally been produced in batch reactors, and it is custom to tailor the synthetic routes to work well in these reactors instead of using reactor set ups designed to handle the relevant chemistry. This results in time-consuming production processes that often need expensive storage of reaction intermediates as well. As such, batch production also implies that the full benefits of the Process Analytical Technology (PAT) initiative of the FDA cannot be realized in the pharmaceutical production process. In contrast, a continuous production environment may potentially lead to improved safety against e.g. runaway reactions, higher productivity and reduced costs, and reduction or elimination of stocks. The aim of this PhD project is to develop continuous operation units optimized for a certain type of reaction or separation process, ideally preserving flexibility. Such approach should yield a methodology and a set of toolboxes applicable to similar design problems. *Research areas: B, C, D* *Continuous pharmaceutical processes; Product & process modelling; Synthesis, design & analysis; Control, operation & monitoring*

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. *Research area: B, C, E* *Multiscale modelling; Synthesis/design; Integration; Enterprise-wide solution*
Joana de Lima Ramos (JLR)  PROCESS	***Guiding biocatalytic process improvements using engineering evaluation tools*** Biocatalysis is an emerging area of technology and to date few reports have documented the economics or environmental profile of such processes During the development of a biocatalytic process and in particular during its scale-up, there are several required considerations. Two of the most important are the economic and environmental profile. The present project is focused on the development of engineering tools in order to assist a fast and accurate economic and environmental analysis. When applied to a given process these have a decisive role in helping to identify bottlenecks in process development, and to justify where to put effort and resources. Further, to exemplify the methodology, *g*uidelines for the successful biocatalytic production of chiral amines using transaminases will be identified through process economic and environmental assessment. The outcome of the present research will establish new tools and knowledge useful in biocatalysis and (bio-) process development. *Collaborations: Evonik, DSM, Lonza*

Paloma Andrade Santacoloma (PSA)  PROCESS	***Multi-enzyme process modelling*** Nowadays multi-enzyme processes are seen as an alternative to assist in the synthesis of complex compounds of industrial interest. In general, a multi-enzyme in-pot process is characterized by the mixture of enzymes that catalyze several reactions in a single pot. Therefore, the individual enzyme contributes with its specific action to drive a given transformation to the subsequent one until the desired product is obtained. In this manner, purification steps of intermediate products may be eliminated. Consequently, it potentially leads to considerable process improvements like increases in the process yield and reduction in downstream processing and operating costs. The objective of the project is to develop a methodological framework for the mathematical modeling of these processes, integrated with a computer-aided methodology, which enables the analysis of models, simulations, parameter estimation, sensitivity analysis, multi-objective criteria evaluation and the like. The idea is to use the models to find either promising configurations for experimental validation, or, evaluate and analyze an existing process under different conditions by simulation, to identify opportunities for improvement. *Research area: Process technology and units operations*
Noor Asma Fazli Bin Abdul Samad (NAS)  CAPEC-PROCESS	***Control of process operations and monitoring of product qualities through hybrid multi-scale model-based analysis*** A generic multi-dimensional model-based framework of batch crystallization processes has been developed covering a wide range of crystallization models and operational scenarios. In order to control and monitor the crystallization operations and to ensure that the desired crystal size distribution (CSD) is achieved, an appropriate Process Analytical Technology (PAT) system (= set of appropriate monitoring tools + actuators) needs to be designed as well. Therefore the use of the generic model is illustrated through the ICAS-PAT software for design of process monitoring and control systems. ICAS-PAT consists of a model library and a knowledge base that allows the user to design/validate PAT systems through a systematic computer-aided framework. The generic crystallizer model has been implemented in the ICAS-PAT model library. The application of the model-based framework has been tested through a batch cooling crystallization process case studies (potassium dichromate, paracetamol, sucrose etc.) where the objective is to obtain a desired CSD. *Research area: B, C, D* *Modelling framework, generic model; crystallization; process control; product monitoring*

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. *Research area: B, E* *Process modelling; waste-water treatment*
Rui Xue (RXUE)  PROCESS	***Reactor and process design for multi-enzymatic synthesis*** Enzyme cascades (which mimic nature) using two or more enzymes sequentially for the synthesis of useful chemical compounds are attracting increasing interest as a potential means of production. Such schemes overcome many of the conventional problems with integrating biocatalysis including media, temperature and pH swaps. In this way the possibility of improved processes are possible. Likewise improvements the use of enzymatic processes may assist approval in some regulated industries. However the design of such systems lacks a fundamental basis. The objective of this PhD project is to study the design of a multi-enzymatic process using the synthesis of neuraminic acid derivatives as an example.

Yuan Xu (XUY)  PROCESS	***Process technology for lipase-catalyzed biodiesel production*** As one of the products from lipase-catalyzed reactions, biodiesel is one of the most promising renewable energy alternatives. The chemical process of biodiesel production has been well developed but the enzymatic process is still in its infancy. In this project lipase-catalyzed biodiesel production is taken as an example for the next generation of process technology. The reactor and separation technology are the core considerations to improve the process efficiency. The scope of this project is to establish a suitable scale-down methodology to test and accurately predict the performance of a process for effective conversion of oils into biodiesel. A mini pilot-plant (20L) scale is being built and will be evaluated for the feasibility and the robustness of the chosen design. *Collaboration: Novozymes A/S, Emmelev A/S, Aarhus University, DTU management*
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 mixture 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. *Research area: A, B, C* *Tailor-made chemical (blend) products;fuel-blends, blend design methodology; bio- and pharmaceutical products*

3.5 External PhD-students (projects)

Klaus Reinholdt Nyhuus Hansen (KRNH)  DTU Management-CAPEC	***New product introduction for the pharmaceutical industry*** It is well known, that the pharmaceutical industry is struggling with increasing cost and length of R&D projects. Earnings of a drug drop drastically after patent expiration. Thus, the industry spends much effort on reducing Time-to-Market. However, a suitable methodology for planning operations immediately prior to launch is especially lacking. Due to strict cleaning requirements, production setups are very long. Production volumes are thus large and intermittent and the entire supply chain becomes rigid and inflexible. Besides forecast uncertainty, which is difficult for new products, other risks and uncertainties from carrying out reimbursement negotiations with authorities in each market e.g. reimbursement levels and product price can also disrupt the execution of a market launch. In this project a MILP-based methodology for planning operations before and during market launch is developed, which fits into the S&OP structure of pharmaceutical companies while considering risks and uncertainties. The methodology should be connected to the existing methodologies; pipeline planning, capacity planning and production planning. *Research area: Planning and scheduling; Operations*
Lida Simasatitkul (LDSI)  CU Thailand - CAPEC	***From biomass to fatty alcohol via bio-diesel: Optimal process design*** The objective of this project is to develop a systematic step by step methodology to obtain flexible process flowsheets for biodiesel and related products from different bio-sources. The methodology will generate different flowsheet alternatives, analyze them through process simulation and evaluate them based on operational issues, economics, and supply chain as well as sustainability measures to determine the best process design. The systematic methodology will be applied to a case study to determine the optimal process design to produce a combination of at least two products: bio-diesel and/or fatty alcohol from at least two different bio-sources: palm oil and waste cooking palm oil. The process flowsheet should be flexible to allow the processing steps required for both the products using both the raw material sources. The process design should be flexible so that changing prices/supply of raw materials as well as prices/demand of products can be handled. That is, the process flowsheet should be able to handle the changing operating conditions for the raw material to product processing routes. Collaboration with Chulalongkorn University, Bangkok, Thailand (Prof A. Arpornwichanop) *Research areas: Process design, modelling, simulation, analysis*

3.6 Other collaborations

Computer aided design of ionic liquids (B. C Roughton, PhD-student; Prof Kyle Camarda, University of Kansus, USA)

The objectives of this PhD-project is to create a database with all ionic liquids that can be formed through the available groups, predict the properties of these ILs, and extend the group parameter tables to predict properties of those ionic liquids that could not be handled because of the missing group parameters. Due to the large number of potential ionic liquids that can be already formed, it is expected that this database can be used to identify and select ionic liquids with desired (target) properties, as well as to find new properties to be modelled that will be necessary for a wider range of applications of ionic liquids. In this way, the created database of existing and new ILs will be equipped with a search engine to quickly identify the needed IL, if it exists. A database has been created with known and generated ILs; property estimation methods have been collected and tested; a search engine for selection of ILs based on target properties has been developed (PEC10-17).

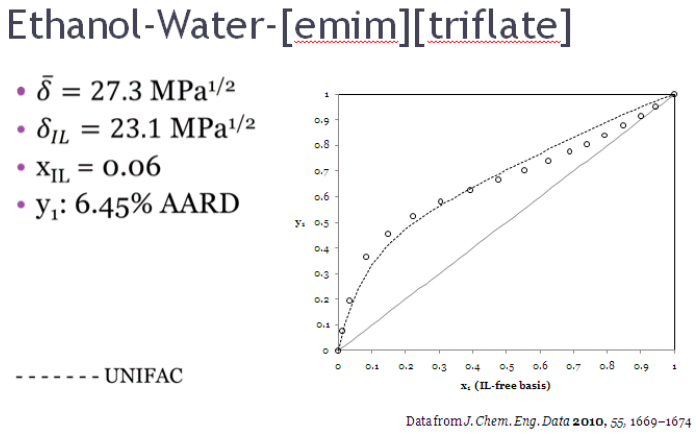


Figure 3.1: Breaking the ethanol-water azeotrope with an ionic liquid

Methodology and algorithm for design and synthesis of reactive distillation columns (Amnart Jantharasuk, PhD-student; Prof Suttichai Assabumrungrat, Chulalongkorn University, Bangkok, Thailand)

The objective of this work is to develop a methodology for design and analysis of reactive distillation columns for multicomponent reactive systems. The concept of driving-force and reverse design approach will be combined to determine near-optimal designs with respect to energy consumption, waste and cost. Hengstebeck's procedure for reduction of multicomponent systems to binary systems will be adapted to "elements" so that multi-element reactive systems can also be reduced to binary element systems. From the binary reactive element driving force and vapor-liquid phase (reactive) diagrams, the already established methods for distillation design will be applied. Here, the driving-force diagram will first be used to identify the location of the maximum driving force (according to the driving force concept, larger driving force implies better separation, less waste, less energy consumption and therefore, lower cost). The reverse approach helps to determine the design of the distillation column that matches the target driving force. Once the reactive distillation

design has been obtained, it will be validated with rigorous reactive distillation models and then, if feasible, through experiments. Details of the developed methods and tools can be found in PEC10-49.

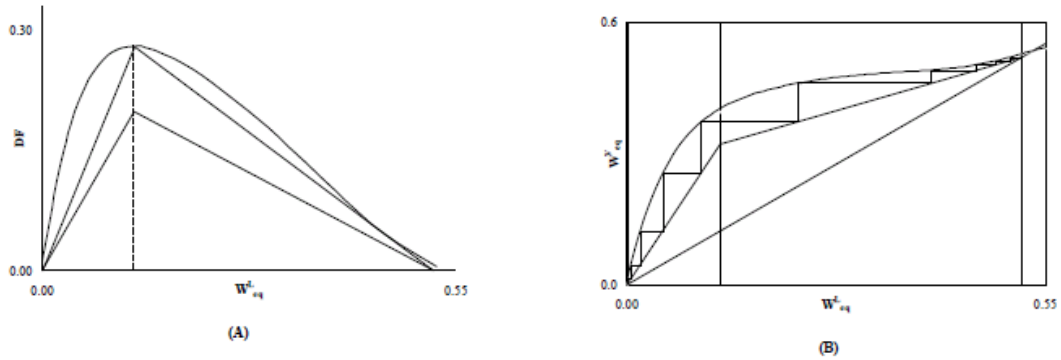


Figure 3.2: Reactive phase diagrams for methyl acetate synthesis. A- element driving force diagram; B- element reactive equilibrium diagram

Computer aided flowsheet design using group contribution methods (Susilpa Bommareddy, PhD-student; Prof Mario Eden, Auburn University, USA)

There are many different approaches to process synthesis including expert systems, optimization or algorithmic methods, and conceptual methods based on physical insights. The objective of this project is to develop a novel hybrid method for Computer Aided Flowsheet Design (CAFD) technique that combines physical insights with algorithmic reverse design approaches to enable systematic identification of feasible flowsheets at significantly reduced computational expense. The framework CAFD is based on the process group (PG) contribution approach developed by d'Anterroches and Gani (2005). The CAFD approach is inspired by the group contribution based methods for Computer Aided Molecular Design (CAMD), which includes building blocks (atoms and functional groups) to generate and represent molecules; group contribution (GC) based property models to predict target properties; a standard molecular structure notation system (such as SMILES) to store and visualize the molecular structure information; and a synthesis method to generate and screen molecules that match the target (design) properties. Analogous to CAMD, in the CAFD approach, flowsheets are generated and represented by functional process groups; process group contribution based property models are employed to predict flowsheet properties; a notation system (called SFILES) is used for storing the flowsheet structural information; and a synthesis method is used to generate and identify the feasible flowsheets. Like functional groups in molecules that are characterized by atoms and their molecular weight, each process group is characterized by the type of unit operation/process and their corresponding driving force. Given the wide range of unit operations that could potentially be used, a flexible and systematic CAFD framework is needed to automate the formulation, analysis and solution of the flowsheet synthesis/design problem. The framework being developed in this work serves as the architecture for a software implementation and incorporates efficient screening and selection algorithms for combining the PGs to yield all feasible flowsheet alternatives. Each PG contributes to the flowsheet (performance) properties, which can be calculated once a feasible configuration has been identified. The candidate flowsheets are ranked based on performance criteria like energy consumption, amount (mass) of external agents used and/or cost/profit. Once a set

of near optimal flowsheet alternatives have been identified, rigorous simulation is used to verify the predicted performance and select the best option.

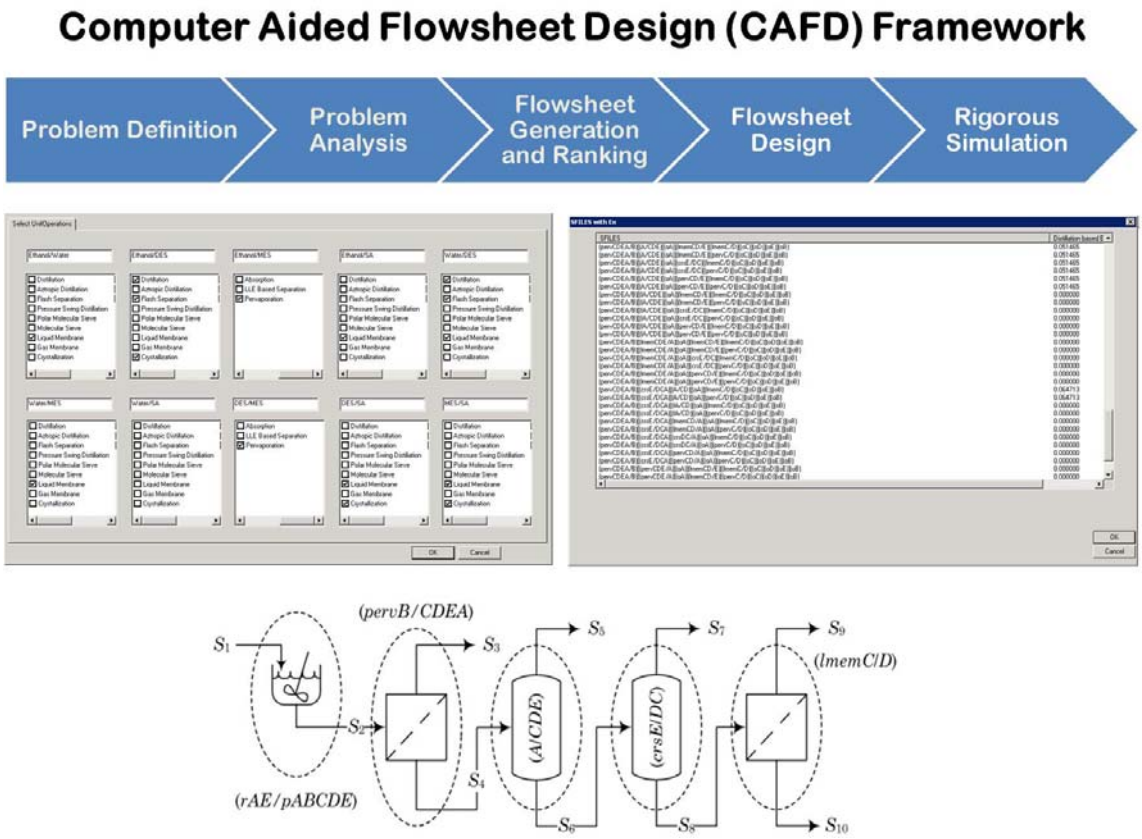


Figure 3.3: Computer aided molecular design (CAMD) versus computer aided flowsheet design (CAFD)

4. CAPEC-PROCESS Software

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

The objective of the CAPEC-PROCESS software is to promote the use of computer aided methods and tools developed by CAPEC and PROCESS in the solution of current and future process/product engineering problems. The CAPEC-PROCESS 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, SSF)
- 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 14.0

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 (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 the new features of the latest version of ICAS. Figure 4.1a highlights the idea of integration and the advantages that can be obtained through this integration.

In ICAS 14.0, new features have been added to the following tools: ProPred (pure component property prediction), MoT (modelling toolbox), ProCamd (computer aided molecular design), and the CAPEC-database. 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, and a solvents database. In addition, three special software (EXCEL based): Sustain-Pro, ICAS-PAT and the Virtual PPD-lab (*v*PPDL) have been revised and improved, while two new software – ECON (software for process economic analysis) and SSF (solvent selection/design for organic synthesis) have been added. 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. In ProCAMD, it is now possible to design the polymer repeat units as well as check for target properties of generated structures through ProPred.

ICAS combines **computational tools** for modeling, simulation (including property prediction), synthesis/design, control and analysis **for chemical products and their processes** in a single **integrated and flexible system**.

ICAS employs algorithms 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.

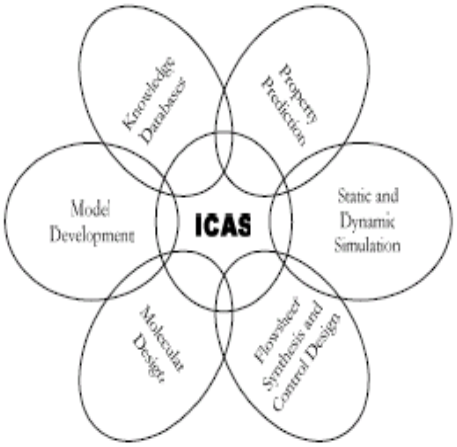


Figure 4.1a: The idea of integration within ICAS

In general, ICAS 14.0 has become a much more robust and reliable version of ICAS with a wider application range. Finally, new additions to ICAS documents related to ProCAFD and Batch-Dis can be found after installation of ICAS under the examples-directory. New versions of manuals for the following tools in ICAS are also available - ProPred, MoT, SoluCalc and ProCamd. After installation of ICAS, users will find a number of worked out examples given in the "examples" and "tutorials" directories. Figure 4.1b shows through a screen-shot of MoT, some of the developed new features while Fig. 4.1c highlights some of the new features in ProPred.

In ICAS 14.0, MoT has new features (work-flows, automation of steps; documentation interface and report generation; Monte Carlo uncertainty analysis; confidence interval calculation; plot of sensitivity functions; improved dynamic parameter estimation; discretization of coupled PDEs); ProCamd has new fatures (selection compounds by number; show compounds, which are in database, not in database, and all compounds; use of the Dortmund UNIFAC model; property description on Mixture page; running ProCAMD with predefined properties) and ProPred have had a major revision with new parameters for the MG and CI methods, new properties as well as uncertainty estimates (see Fig. 4.3). Also, new filled parameter tables are given for the UNIFAC and Dortmund-UNIFAC models. EXCEL-based macros (SustainPro; CAPECdatabase and vPPD-lab) have also been improved.

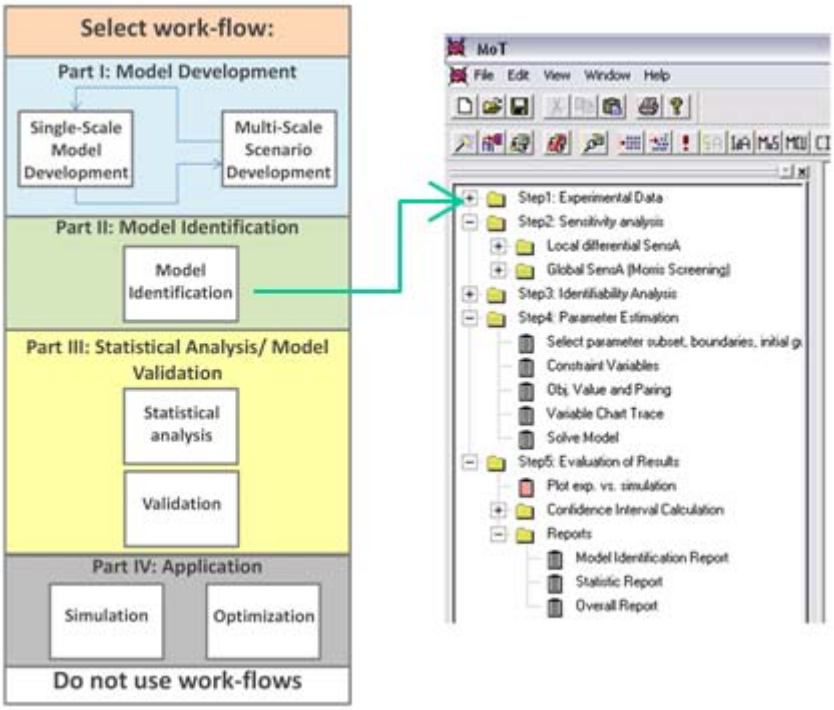


Figure 4.1b: Screen-shot from ICAS-MoT highlighting some of the new features.

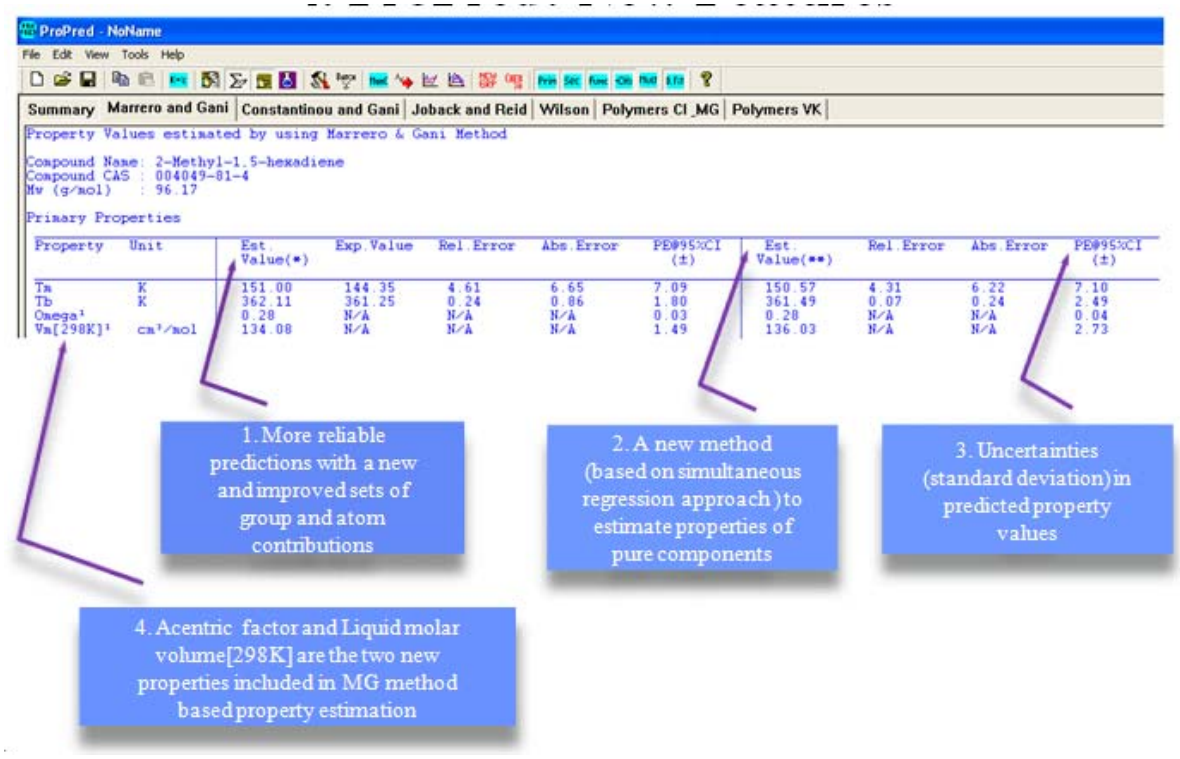


Figure 4.1c: Screen-shot from ProPred highlighting some of the new features in ProPred

4.2 EXCEL based macros (ProPred, CAPECDB Manager)

Two EXCEL based software has been developed to further 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.

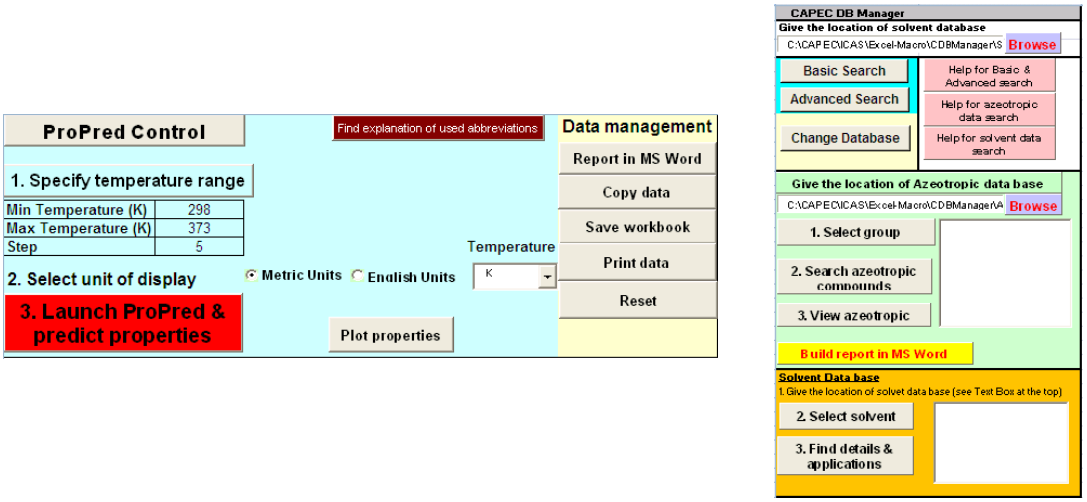


Figure 4.2: EXCEL based macro to run ProPred (left) and CAPECdatabase (right)

4.3 UNIFAC-Utility

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

4.4 ECON (software for economic analysis)

The ECON software has been developed in visual basic for applications related to economic analysis. ECON provides the following options.

- Equipment cost calculation
- Capital cost calculation
- Operating cost calculation
- Economic analysis
- PIE chart analysis
- Sensitivity analysis
- Comparison of design alternatives

The cost calculations in ECON are primarily based on the cost models given in *"Plant Design and Economics for Chemical Engineers" (Peters and Timmerhaus, 2004).*

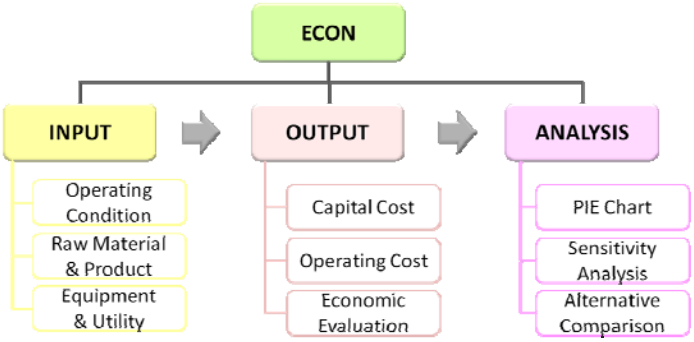


Figure 4.3: Structure of the ECON software

4.5 Special ICAS-based software (ICAS-PAT, SustainPro, vPPD-lab)

4.5.1 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 PEC09-06). A manual and several solved case studies are available. Figure 4.4a highlights the main features of ICAS-PAT.

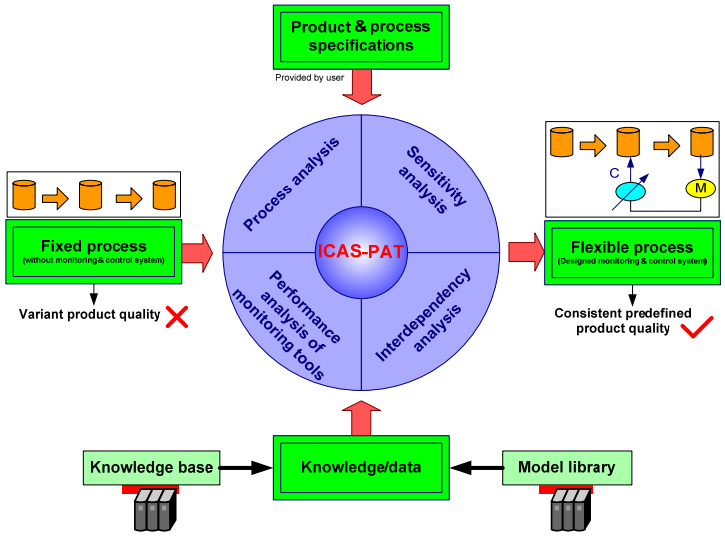


Figure 4.4a: Overview of the main features of ICAS-PAT.

4.5.2 SustainPro

SustainPro is an EXCEL based software, which provides options for retrofit analysis and performance analysis of a given process. As highlighted in Fig 4.4b, 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 4.4b, 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.

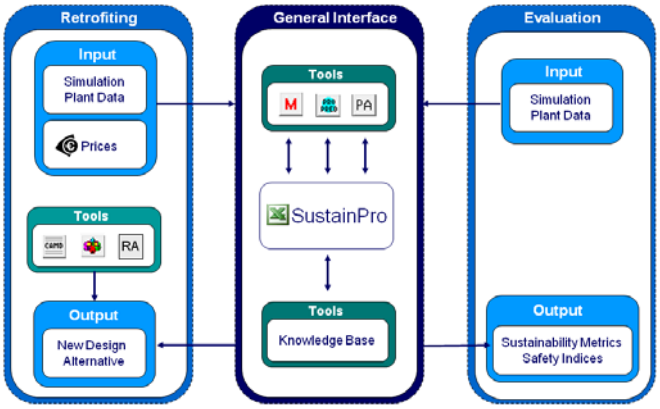


Figure 4.4b: Overview of the main features of SustainPro

4.5.3 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.). The above ideas are organized through a framework for efficient management of the complexity. Figure 4.4c gives an overview of the main features of the *v*PPD-lab software, which has been used in the design and evaluation of the controlled release of a drug active ingredient (codeine) through a polymeric microcapsule. In the first step the problem is defined (identity of the active ingredient; the desired controlled release parameters, etc., are given in the "documentation" box of *v*PPD-lab). In the second step the selection of the application source (codeine released into the body), the primary properties of solvent and the polymer (needed by the controlled release model) is made (if the user is unable to provide this information, methods for solvent design and polymer design are used to generate a list of candidates to select from). In the next step the selection and calculation of the functional properties needed to evaluate the controlled release design is made (if models are not available, the modelling software helps to generate new models). In the next

steps, the product performance model is used to predict the product behaviour. If the desired (target) performance is matched, then the last step of verifying the product performance through experiments is performed. If the target is not matched, it is possible to repeat from any of the earlier steps with a new design alternative. An option for formulation design together with the associated databases has been added.

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

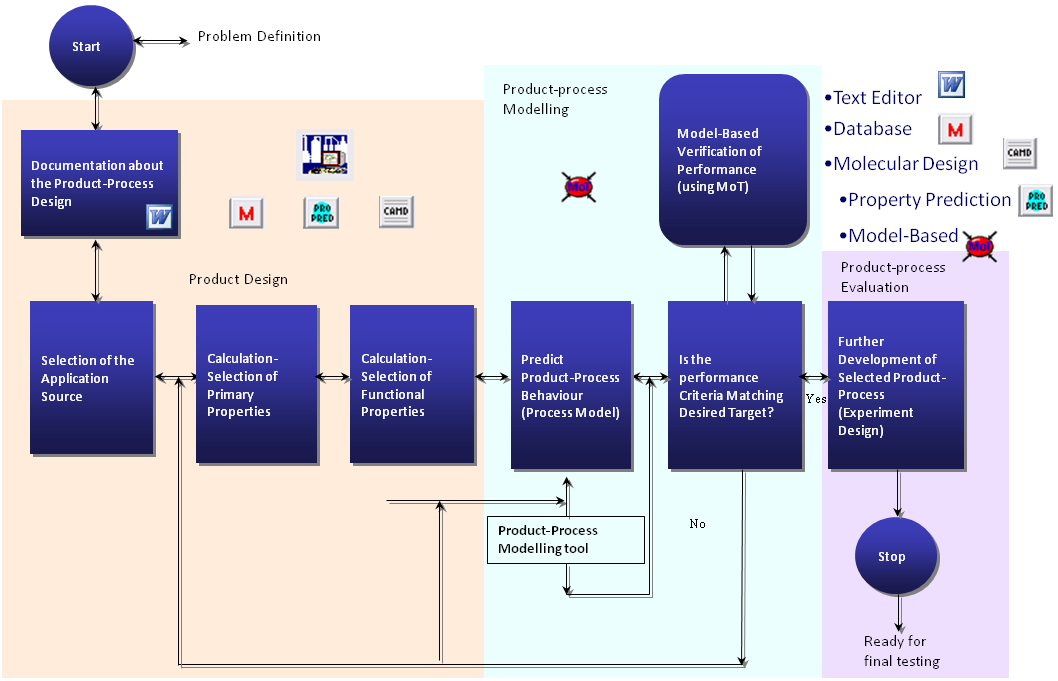


Figure 4.4c: The virtual product-process design lab

4.6 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:

I. *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).

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

4.7 Solvents Selection Framework (SSF)

This software provides a solvent selection framework for all solvent-related problems. The current version is developed as a prototype to implement/test the solvent selection/design method for organic synthesis of Gani et al. (Computers & Chemical Engineering, 32(10), 2420-2444, 2008). It uses ProPred, ProCAMD, the CAPEC database and a special solvents database. The software guides the user through the different steps of the algorithm, extracts the necessary data and/or calculates them by calling ProPred. Once the solvent selection problem has been defined, SSF calls ProCAMD as well as searches the common solvents database, and orders the list of feasible solvents for each reaction. In this way, for multiple reaction systems, a matrix of solvent candidates is obtained.

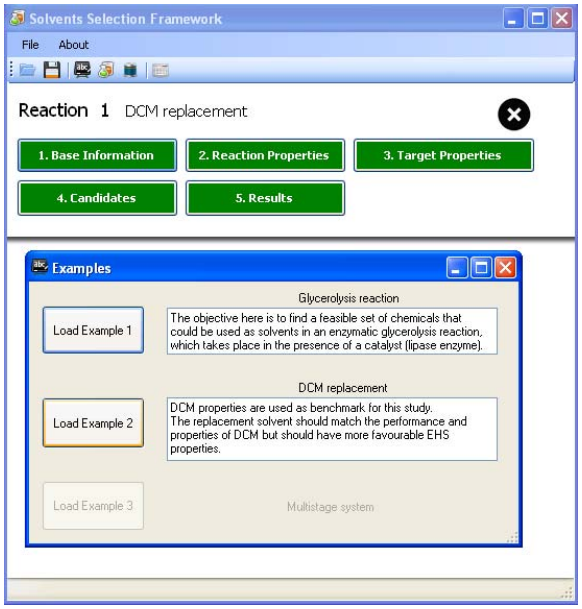


Figure 4.5: Solvent selection for organic synthesis through SSF

4.8 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.

5. Research highlights (2010-2011)

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 Development of group contribution^{plus} models for prediction of properties of organic chemical systems – Merlin Alvarado-Morales (PEC10-13)

This PhD-project was concerned with the development and application of a framework for synthesis, design and analysis of chemical and biochemical processes. The developed framework addressed the formulation, solution, and analysis of the synthesis/design problem through a systems approach where emphasis was given on the use of the process-group contribution based methodology. This methodology helps to generate and test process flowsheet alternatives in a truly predictive manner, in the same way, molecules are designed through group contribution based computer aided molecular design.

The three fundamental objects of the PGC-methodology are the process-groups (building blocks) representing process unit operations; connectivity rules to join the process-groups, and the flowsheet property models to evaluate the performance of the generated flowsheet structures. In order to extend the application range of the PGC methodology, a set of new process-groups together with their specifications have been developed. The synthesis of the chemical and biochemical process flowsheets has been performed through the reverse property approach, where the process-groups are combined to form feasible flowsheet structures having desired (target) properties. The design of the most promising process flowsheet candidates is performed through the reverse simulation approach, where the design parameters of the unit operations in the process flowsheet are determined from the specifications of their inlet and outlet streams inherited from the corresponding process-groups. The reverse simulation methods supporting the framework are based on the attainable region (AR) and the driving force (DF) concepts, which guarantees a near optimal performance design with respect to selectivity for reactor units and with respect to energy consumption for separation schemes.

The framework for synthesis and design of chemical and biochemical processes together with the models, methods and tools is generic and can be applied to a large range of problems, either to improve an existing process flowsheet or to design a new process flowsheet. The developed framework and associated computer aided methods and tools have been tested using a series of case studies, for example, the production of ethanol, succinic acid and diethyl succinate from renewable resources.

5.1.2 Innovation in integrated chemical product-process design: Development through a model-based systems approach – Elisa Conte (PEC10-28)

The ‘consumer oriented chemicals based products’ such as shampoos, sunscreens, insect repellents are used everyday by millions of people. They are structured products, constituted of numerous chemicals. This complexity gives the reason for which mainly experimental techniques are still employed in the design and verification of such products. The objective of this project is to tackle the problem with computer-aided tools at first, using experimental techniques for final testing, evaluation and amendment. In this way,

time and resources can be spared and the product can reach the market faster and at a reduced cost.

The main contribution of this project is the development of an integrated methodology for the design and verification of formulated products. The methodology includes a first stage in which computer-aided techniques are employed to reach the base case product formula, a second stage in which experiments are planned and a third stage in which experiments are performed to reach the final product formula.

The main focus of the project is on the development of the computer-aided stage of the methodology described above. The methodology considers two different scenarios: the design of new products and the verification of modified and/or existing products. In the design scenario thousands of alternatives need to be considered since the identity of the ingredients is unknown, therefore the problem assumes explosive combinatorial potential and short cut methods are necessary. In the verification scenario, a shortlist of candidate ingredients is provided, therefore the problem size is much smaller and rigorous property models can be employe and/or developed.

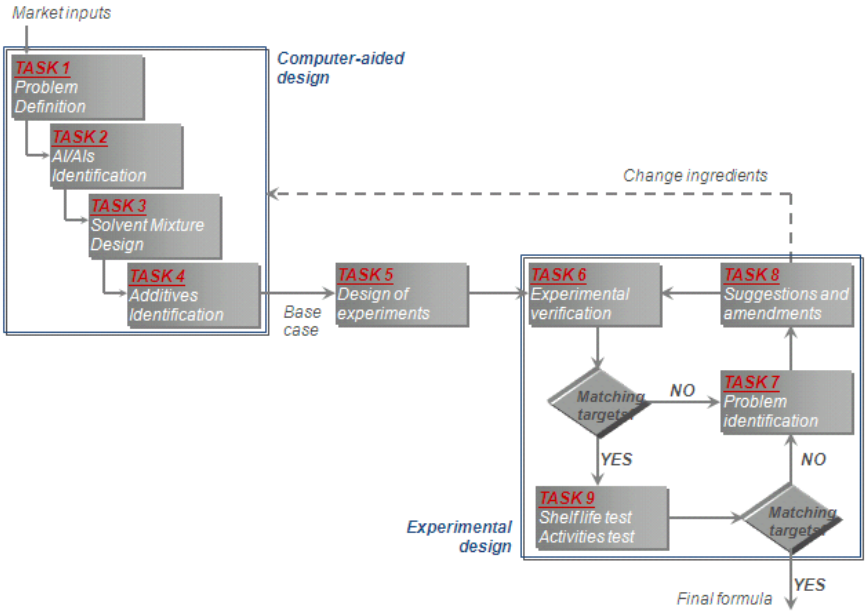


Figure 5.1: Systematic methodology for formulation design and verification (Elisa Conte)

When using computer-aided tools for product design, several issues need to be addressed: new property models may need to be developed and/or the application range of existing property models may need to be extended (new model parameters are needed), new and more efficient methods and tools for the application of the models may need to be developed, together with flexible frameworks which collect the methods and tools and allow to use them in an integrated way. All these issues are addressed in this work: new property models for the estimation of the target properties are developed; two algorithms for the design of binary mixtures and for the stability test of liquid systems are built, together with the corresponding computer programs; the computer-aided stage of the methodology for formulation design and verification is included in the environment of the in-house software the 'virtual Product-Process Design laboratory'.

Four case studies have been developed to illustrate the use of the proposed methodology.

For two of these case studies the complete methodology has been applied, that is, including the stages of experimental planning and experimental testing/amendment. For the other two, only the computer-aided stage has been faced.

5.1.3 Continuous Culture Microbioreactors - Daniel Schäpper (PROCESS 2010)

Effcient fermentations at industrial scale are usually preceded by an enormous amount of research work aimed at optimizing the productivity of the strain in question. Before that, the question of the selection of the correct strain already accounts for a substantial amount of work. Today, most screening is done in microtiterplates which allow for cultivations similar to those in shake asks, however, due to the much smaller volume, microtiterplates are much more streamlined for parallel, machine-controlled operation. Out of these cultivations, a number of strains are selected for further investigation, which typically means performing cultivations in larger and larger scales. As the size of the reactor increases from shake ask to bench-scale reactors to pilot-plant installations the number of strains decreases until only one strain is left at production scale which hopefully is the ideal strain. However, precisely this scaling-up can give problems, as strains may behave differently in a shake ask than in a production scale reactor. There is therefore a need for a small-scale production platform which can offer more reliable upscaling; Or in other words a platform which is better at mimicking full-scale operation is needed. Apart from the fermentation industry, research also depends on well-controlled cultivations with tight measurement and control in order to obtain meaningful data about the strain metabolism.

Microbioreactors have the potential to be the platform needed to fulll the above requirements: The working volumes are relatively small, typically < 1 mL, and they can be operated in different operating conditions such as batch or continuous cultivations. Additionally, their small size offers a number of possibilities: Under the presence of good mixing, one can assume the contents of a microbioreactor to be free of gradients (e.g. nutrients, oxygen) which allows for a precise determination of the state of the cultivation. Additionally, the large surface to volume ratio opens up the possibility for quick changes in temperature, so that e.g. the inuence of step changes on the metabolism can be investigated. The advance of miniature online measuring techniques makes it possible to measure at least the basic culture variables such as dissolved oxygen (DO), cell density (OD) and pH continuously and without disturbing the cultivation. Online measurements are at this scale very susceptible to the presence of bubbles|as is a microbioreactor itself as already small bubbles can disturb the flow in microchannels. Bubble-less aeration through a membrane elegantly solves both problems and also separates the broth from external inuences.

The microbioreactor developed here was designed to fulfill the above requirements; Additionally, much focus was put on the single-use aspect. This includes both being cheap in fabrication and in operation, and also requires the reactor to be sterilizable by industrial methods. It consists entirely of polydimethylsiloxane (PDMS) and contains two optical sensor spots for the measurement of DO and pH as well as a micro-stirrer for agitation of the broth. It has previsions for the measurement of cell density (by means of optical density measurent) as well as membrane aeration. Both temperature and pH can be controlled online and automatically.

The device has outer dimensions of 14 mm diameter and 4.2 mm height. The reactor chamber is a cylinder with 8 mm diameter and 2 mm height resulting in a culture volume of 100 μL. The uidic connections are done by piercing the reactor side walls with needles - the

PDMS will tightly enclose the needle to prevent leakage. The reactor chamber is sealed with a semi-permeable membrane (thickness approximately 80 μm), through which the gases can diffuse. Both oxygen and off-gases are exchanged this way. Additionally, pH can be controlled by the addition of CO_2 or NH_3 to the aeration gas ow to lower or increase pH respectively. The density of the culture broth is measured by a transmittance measurement|light is shone through 0.5 mm of culture broth, and the intensity of the transmitted light is measured. This gives an indication of the amount of cells in the broth. Both DO and pH are measured with uorescent sensor spots: Oscillating light is shone onto the sensor spots which in turn emit oscillating uorescent light with a certain phase shift respective to the exciting light. This phase shift relates to the DO or pH of the broth, respectively.

Mixing is solved by means of a small magnetic stirrer bar which, contrarily to what is seen in other microbioreactor solutions, rotates freely within the reactor. Experiments had shown that a stirrer bar rotating in the middle of the reactor will only force the broth into a swirling motion where the outer edges of the reactor do not have enough updraft anymore. The freely spinning stirrer bar however will hit the wall and ricochet chaotically into the reactor chamber again. Thus, over time, all of the reactor oor will be covered which prevents the formation of dead zones.

Temperature is controlled by means of an external (and thus re-usable) heating plate which contains both a temperature sensor and a resistance heating wire. As the oor of the microbioreactor only consists of a membrane which offers virtually no heat resistance, this allows for a precise control of the broth temperature.

In order to provide benchmarking data to be able to evaluate the reactor performance, batch cultivations were done in both shake asks and bench-scale reactors. Finally, corresponding cultivations were performed in the microbioreactor.

Additionally, as an entirely theoretical case study of something completely new, the application of the topology optimization methodology on microbioreactors and the resulting gains in productivity was studied.

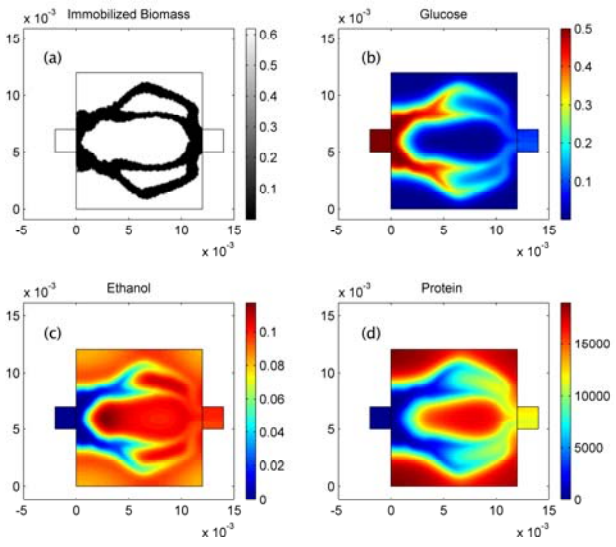


Figure 5.2: Evaluation of the micro-reactor (D Schäpper)

5.1.4 Analysis of Multivariate Sensor Data for Monitoring of Cultivations - Nanna Petersen Rønnest (PROCESS 2010)

Improved monitoring of cultivations has the potential to increase process understanding, enable immediate quality assessment, improve process control, and facilitate optimization of the process. Over the past decades various advanced sensor technologies have been developed, which can facilitate rapid estimations of important biological or chemical variables in the cultivation processes. Despite a large number of academic studies, most of the advanced sensors have not found widespread use in the industry until now. The main aim of this thesis has been to address this apparent discrepancy. The thesis consists of four case studies, which have provided critical evaluations of various sensor technologies and have served to elucidate some of the specific challenges of advanced sensor application in filamentous and industrially relevant cultivation processes.

The first two case studies were focused on quantification of filamentous morphology using off-line laser diffraction and the relation of the size distribution to the rheological properties of the cultivation broth. Firstly, the method of laser diffraction was compared to simple image analysis for quantification of clumps and pellets in *Streptomyces coelicolor* cultivation broth. The laser diffraction technique and image analysis yielded size distributions with similar shape, i.e. unimodal or bimodal distributions. The two techniques produced similar estimations of the population means, whereas the estimates of the standard deviations were generally higher using the laser diffraction technique compared to image analysis. In the second study, laser diffraction was used to quantify the morphology in industrial *Aspergillus oryzae* cultivations. Systematic changes in the size distribution were correlated to (1) the change in morphology as the cultivation progressed and (2) the difference in morphologies observed between continuously fed batches and the batches with pulse-pause feeding. Models were calibrated for prediction of the rheological parameters yield stress, consistency index and the apparent viscosity of *A. oryzae* broth based on the size distribution. Validation on an independent test set yielded a root mean square error of 1.20 Pa for the yield stress, 0.209 Pa s_n for the consistency index and 0.0288 Pa s for apparent viscosity, corresponding to R_2=0.95, R_2=0.94, and R_2=0.95 respectively.

In the third case study, in situ NIR spectroscopy was evaluated for quantification of of two important analytes: glucose and ammonium in *S. coelicolor* batch cultivations. In order to critically evaluate the ability of NIR to measure the two specific analytes, the inherent correlations in the batch process were broken by the use of semi-synthetic samples measured in situ. In addition, samples were collected and analyzed using off-line NIR, to highlight the speci_c challenges of in situ monitoring. The results showed that both off-line and in situ NIR are suitable for the measurement of glucose concentration in the range 1-40 g/L. Using in situ NIR spectroscopy, a prediction error or 1.1 g/L glucose was obtained corresponding to 5.4 % of the mean value in a validation batch. For measurement of ammonium in the concentration range 40-110 mM, a large increase in prediction error was observed for in situ measurements (RMSEP= 11 mM corresponding to 16% of the mean value) compared to off-line measurements (RMSEP = 5.1 mM corresponding to 7.1 % of the mean value). This may be partly explained by a reduction in usable wavelength regions in the in situ NIR spectra compared to the spectra collected off-line, as well as increased noise in the in situ measurements.

In the fourth case study, multi-wavelength uorescence, scanning dielectric spectroscopy (DE), on-line turbidity (OD), and simple software sensors were evaluated for the on-line

estimation of biomass concentration in *S. coelicolor* fed-batch cultivations. The experiments were designed to imitate an industrial process development, thereby introducing significant variation in the process parameters. In this highly challenging system, it was shown that the more advanced sensors with multivariable output did not improve predictions of dry cell weight compared to the more simple measurements of dual frequency DE, on-line turbidity and measurements of carbon dioxide evolution rate (CER). However, the predictions of dry cell weight were greatly improved by combining selected sensors. Thus a prediction error of 1.5 g/L, corresponding to 6 % of the covered biomass range was obtained by using a combination of dual frequency DE, on-line OD and CER measurements. Furthermore, the use of multiple sensors enabled supervision of the predictions in real-time, facilitating an operator intervention such as a change between individual sensors or the collection of an off-line sample for recalibration. It was thereby demonstrated that the on-line biomass sensors fulfill the demanding requirements of process development and can be of great industrial use in both pilot plant and/or industrial production scale.

5.1.5 Continuous Membrane Microbioreactor for Development of Integrated Pectin Modification and Separation Processes - Muhd. Nazrul Hisham Zainal Alam (PROCESS 2010)

Microbioreactor technology has recently made significant progress, and has also demonstrated significant advantages for assessing biological processes over other low cost micro-scale devices such as microtiter plates, microtubes, etc. Microbioreactors (i.e. typical volume < 1 mL) are usually integrated with on-line sensors and actuators, and can often be designed such that they can mimic the events typically taking place in a benchscale reactor system. In this work, a continuous membrane microbioreactor system was developed to facilitate integrated pectin modification and separation processes. The increasing need for high-throughput experimentation in novel 'biorefining' type of processes (e.g. enzyme-catalyzed degradation of complex biopolymers for obtainment of value-added oligosaccharides) justified the selection of the micro-scale reactor.

During the development of the membrane microbioreactor, relevant membrane microbioreactor design parameters i.e. reactor operating feature and size, reactor mechanics (materials, fabrication, membrane separation design, and mixing), reactor fluidics (connections, pumping mechanisms, and feeding strategy), process control of physical parameters (temperature, pH, and pressure) and detection methods for measuring the product concentration were carefully evaluated and implemented. Subsequently, hypotheses formulated for the thesis were tested one by one.

The membrane microbioreactor prototype developed here was realized as a loop reactor system to operate in *crossflow* filtration mode. It was also designed to work under bubble-free conditions with constant volume ($dV_r/dt = 0$). The reactor has outer dimensions of 35 mm (length) x 20 mm (width) x 8 mm (thickness) with an internal working volume of approximately 200 µL. A regenerated cellulose membrane was sandwiched between alternate poly(methylmethacrylate) (PMMA)-polydimethylsiloxane (PDMS) layers achieving a *clamp and play* reactor configuration. Mixing was accomplished with a magnetically actuated stir-bar combined with a high velocity recirculation flow in the loop delivered via a micro-gear pump. The quality of mixing was checked with a simple tracer test by using a fluorescence dye. Complete mixing (i.e. indicated by uniform colour spread of the fluorescent dye) at a system residence time of 1 hour was attained in about 3 minutes

15 seconds. Fluidic connections were established by using standard chromatography fittings, thus providing a *plug and play* fluidic connection design. The reactor has the capacity to operate either in continuous or semi-continuous (i.e. alternate substrate-buffer feeding strategy) mode, and the necessary pressure for the separation to occur was achieved via the feeding pump.

In addition, the prototype was equipped with an on/off temperature control loop where embedded resistance wires were used as the heating element. It was shown that integrated resistance wires coupled to a simple on/off controller result in accurate control of the temperature of the reactor (± 0.1 ^{o}C of the set point value) and provide a good disturbance rejection capability (corrective action for a sudden temperature drop of 2.5 ^{o}C at an operating temperature of 50 ^{o}C takes less than 30 s). A gaseous pH control strategy was also evaluated where the dosing of CO_2 gas and an NH_3 (20 000 ppm) - N_2 gas mixture was used to respectively decrease and increase the pH of the reactor content.

Although the performance of the gaseous pH control method established was satisfactorily (i.e. accuracy of ± 0.1 pH units of the pH set point was achievable), implementation was impeded due to the limited dynamic measurement range of the pH optodes used (i.e. rather insensitive in the low pH range of 4 to 5). In the current membrane microbioreactor design, pH is therefore controlled by adding buffer to the medium.

The functionality of the membrane microbioreactor prototype was further evaluated in biologically relevant experimental work. Here, pectin lyase was employed to catalyze the sugar beet pectin (i.e. 60% methylated, 19% acetylated) degradation process. Results attained demonstrated the workability of the prototype for an extended enzymatic reaction – evaluated under different experimental conditions i.e. molecular weight cut-off (MWCO), reactor residence time, etc. – and showed its usefulness in obtaining real-time process data of the enzyme-catalyzed degradation of pectin. In the benchmarking step, it was shown that reaction conditions applied in the microbioreactor prototype can also be reproduced in the bench scale reactor system – evident by comparable process data (i.e. kinetic profiles) obtained in both scales.

The thesis is concluded with a brief discussion on the advantages and drawbacks of the continuous membrane microbioreactor system developed in this work. Future recommendations on how to further improve the reactor design are included as well, such that the technology can be pushed to meet satisfactorily industrial standards.

5.1.6 Model-based integrated process design and controller design for chemical processes – Mohd. Kamaruddin Abd Hamd (PEC11-02)

This PhD-project was concerned with the development and application of a new systematic modelbased methodology for performing integrated process design and controller design (*IPDC*) of chemical processes. The new methodology is simple to apply, easy to visualize and efficient to solve. Here, the *IPDC* problem that is typically formulated as a mathematical programming (optimization with constraints) problem is solved by the so-called reverse approach by decomposing it into four sequential hierarchical sub-problems: (i) pre-analysis, (ii) design analysis, (iii) controller design analysis, and, (iv) final selection and verification. Using thermodynamic and process insights, a bounded search space is first identified. This feasible solution space is further reduced to satisfy the process design and controller design constraints in sub-problems 2 and 3, respectively, until in the final sub-

problem all feasible candidates are ordered according to the defined performance criteria (objective function). The final selected design is then verified through rigorous simulation.

In the pre-analysis sub-problem, the concepts of attainable region and driving force are used to locate the optimal process-controller design solution in terms of optimal condition of operation from design and control viewpoints. The targets for the designcontrol solution are defined at the maximum point of the attainable region and driving force diagrams. Defining the targets at the maximum point of the attainable region and driving force diagram ensure the optimal solution not only for the process design but also for the controller design. From a process design point of view at these targets, the optimal design objectives can be obtained. Then by using the reverse solution approach, values of design-process variables that match those targets are calculated in Stage 2. Using model analysis, controllability issues are incorporated in Stage 3 to calculate the process sensitivity and to pair the identified manipulated variables with the corresponding controlled variables. From a controller design point of view, at targets defined in Stage 1, the sensitivity of controlled variables with respect to disturbances is at the minimum and the sensitivity of controlled variables with respect to manipulated variables is at the maximum. Minimum sensitivity with respect to disturbances means that the controlled variables are less sensitive to the effect of disturbances and maximum sensitivity with respect to manipulated variables determines the best controller structure. Since the optimization deals with multicriteria objective functions, therefore, in Stage 4, the objective function is calculated to verify the best (optimal) solution that satisfy design, control and economic criteria.

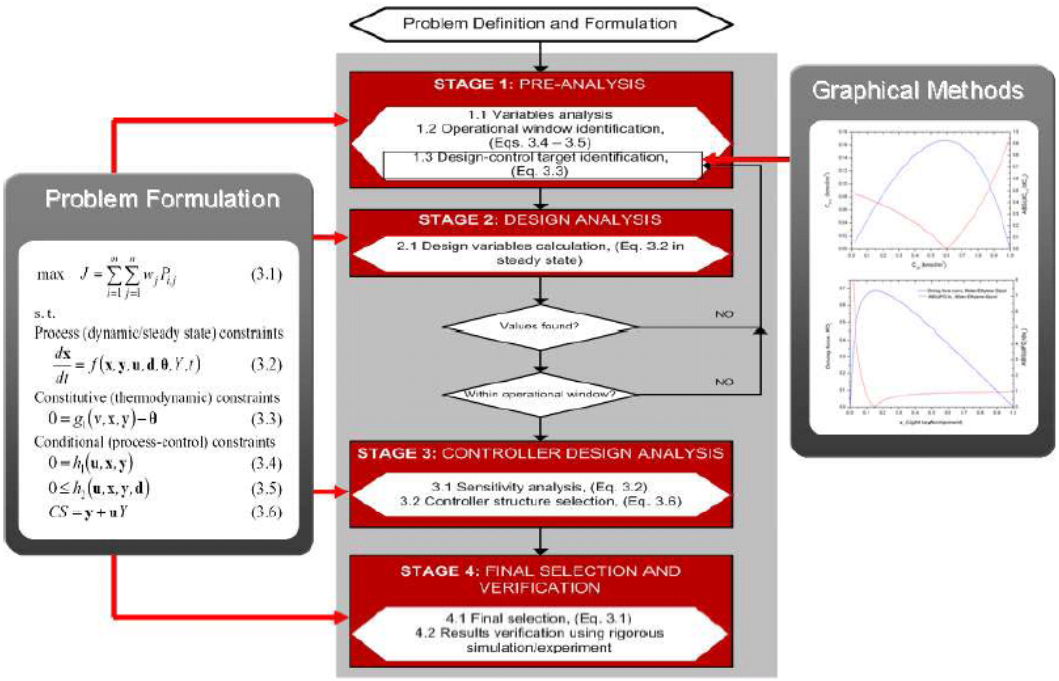


Figure 5.3: Algorithm and software architecture for integrated process design and control (MKA Hamid)

From optimization point of view, solution targets at the maximum point of the attainable region and driving force diagrams are shown the higher value of the objective function, hence the optimal solution for the *IPDC* problem is verified. While other optimization methods may or may not be able to find the optimal solution, depending on the performance of their search algorithms and computational demand, this method using the

attainable region and driving force concepts is simple and able to find at least near-optimal designs (if not optimal) to *IPDC* problems.

The developed methodology has been implemented into a systematic computer-aided framework to develop *ICAS-IPDC* software. The purpose of the software is to support engineers in solving process design and controller design problems in a systematic and efficient way. The proposed methodology has been tested using a series of case studies that represents three different systems in chemical processes: a single reactor system, a single separator system and a reactor-separator-recycle system.

5.1.4: Molecular Modeling of Enzyme Dynamics Towards Understanding Solvent Effects – Rasmus Wedberg (PEC11-03)

This thesis describes the development of a molecular simulation methodology to study properties of enzymes in non-aqueous media at fixed thermodynamic water activities. The methodology is applied in a molecular dynamics study of the industrially important enzyme Candida antarctica lipase B (CALB) in water and organic solvents. The effects of solvent on structural and dynamical enzyme properties are studied, and special attention is given to how enzyme properties in organic solvents are affected by the hydration level, which is shown to be related to the water activity.

In experimental studies of enzyme kinetics in non-aqueous media, it has been a fruitful approach to fix the enzyme hydration level by controlling the water activity of the medium. In this work, a protocol is therefore developed for determining the water activity in non-aqueous protein simulations. The method relies on determining the concentration of water in a region of the simulation box far from the protein surface. In order to evaluate the corresponding activity, a previously developed methodology based on fluctuation solution theory is employed to compute the excess Gibbs energy of the water/organic solvent mixture. This requires that separate simulations of this mixture are carried out at different compositions, and that the total correlation function integrals, i.e. spatial integrals of the pair radial distribution functions (RDFs), are evaluated.

A main challenge is that the total correlation function integrals do not converge within the system size of the simulation box generally used in simulation. Therefore, a method is developed for extending the RDFs to arbitrary distances so that the integrals can be evaluated. The method, which was first used in the classical study of the Lennard-Jones fluid by Verlet (Verlet (1968), *Phys. Rev.*, **165**, 201–214), is here extended for application to simulations of molecular fluid mixtures. It extends the RDFs by enforcing that the corresponding direct correlation functions follow a certain approximation at long distances. This approximation is here derived in terms of statistical mechanical fluid theory. An extensive set of numerical tests are carried out for validating the method, and it is found that thermodynamic properties of good accuracy are obtained from the integrals of the extended RDFs. The method is also shown to be at least as good as existing methods for correlation function integration, while for small systems, it seems to be even better.

The method is applied to compute the excess Gibbs energy of the mixtures of water and organic solvents used in the simulations of CALB. This allows to determine the water activity of the simulated systems and thus to compare protein properties in different organic solvents at fixed water activities. The study bridges therefore the previously used simulation approach where properties were compared at similar hydration levels (Yang *et*

al (2004), *Biophys. J.*, **87**, 812–821); Micaˆelo and Soares (2007), *FEBS J.*, **274**, 2424–2436; Trodler and Pleiss (2008), *BMC Struct. Biol.*, **8**) and the approach to fix the water activity which often is used in experimental studies.

The water activity is shown to have a profound effect on the structure and dynamics of CALB. Conformational flexibility, for instance, increases with increasing hydration in acetone, t-butanol, methyl t-butyl ether and hexane, but not in methanol. A consequence of this is that hydration needs to be carefully considered in simulation studies of proteins in organic media. The organic solvent is also shown to affect structure and dynamics of CALB. The effects on flexibility can partially be attributed to the mobility of the hydration water, as proposed in a previous study (Trodler and Pleiss (2008), *BMC Struct. Biol.*,**8**). The present results indicate that flexibility may also be affected by adsorption of organic solvent molecules to the enzyme surface. This seems in particular to be the case in t-butanol in which the lowest flexibility of CALB is observed.

Future applications of the methodology may lead to an improved understanding of enzyme properties in non-aqueous media, which may have significant impact on the development of rational strategies for solvent selection in biocatalysis.

5.2 Publications Record

The last 12-months has seen a big increase for CAPEC and PROCESS in the number of peer-reviewed journal publications. 61 papers from 2010 to present (plus 14 “in press” and another 7 “submitted”) have been published in major chemical engineering journals (see Appendix 7.3 for more details). There have been 11 plenary or keynote lectures in international conferences and 125 (96 in 2010 and 29 until 1 June 2011) presentations have been made in important international conferences. This has given CAPEC and PROCESS greater visibility and attracted more attention to the research results published by both centers. 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 14.0 has all the latest property models and updated property model parameters. Also, during this period, 2 CAPEC published papers received the best paper award, 3 papers received the best poster award and 1 PhD-thesis won the EFCE PhD thesis of Excellence in the area of CAPE.

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 more than 50 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.

6.3 Managing the complexity through a systems approach

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

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

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

The multi-dimensional and multi-scalar nature of problems is highlighted through Fig. 5.1, where, it can be noted that 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.

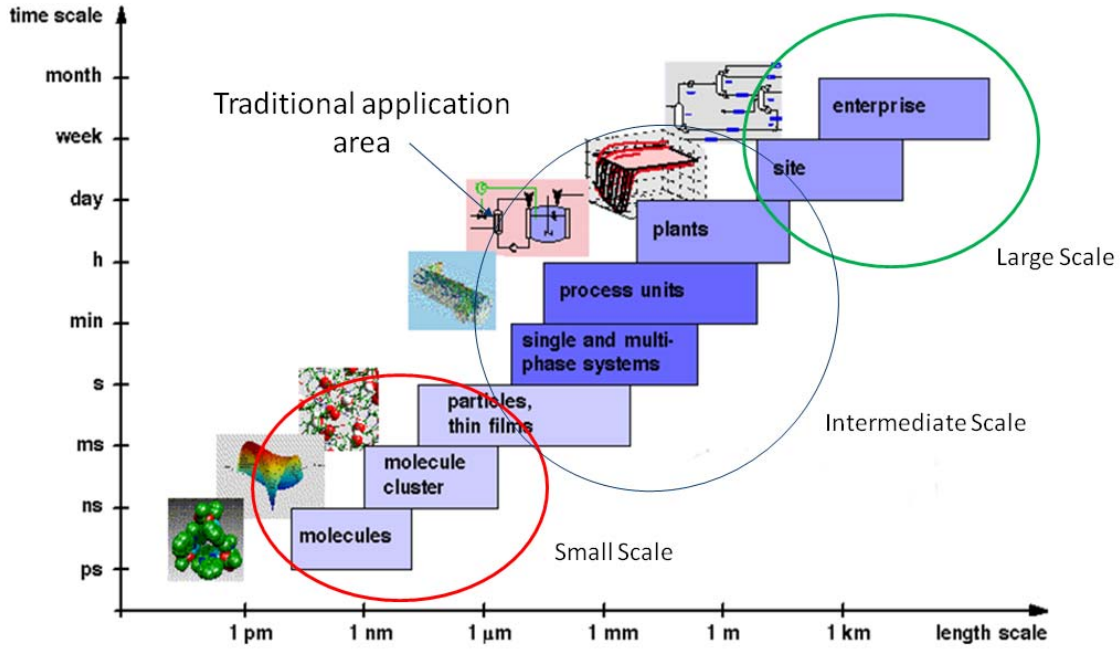


Figure 6.1: Multiscale nature of product-process design problems

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.

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

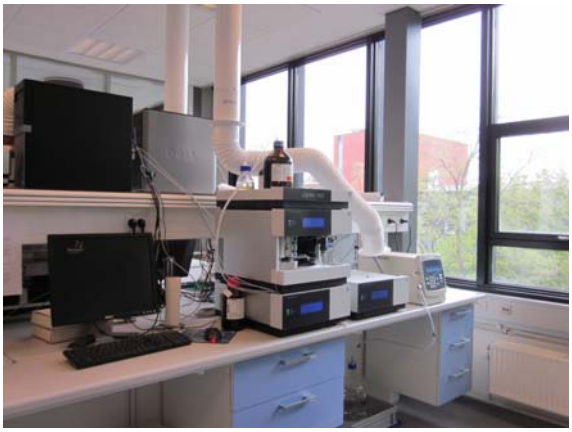
Within the next 6-months, CAPEC and PROCESS plan to jointly start 3-4 PhD projects in the areas of energy and environment; product-process design; multiscale modelling; (bio-) process synthesis and design, design/control under uncertainty; solvent based organic synthesis; and process intensification. Three project proposals have been submitted to the EC-funded FP7 program on model-based control, monitoring and process intensification. Two post-doctoral positions, one in the area of modelling and the other in the area of product design will be started in August-September of this year. Also, several new MSc-level projects on computer-aided product design (crystallization); solvent-based product design; energy and environment; design under uncertainty; sustainable process design; micro-reactor fermentation; cellulose hydrolysis kinetics; and uncertainty quantification in property prediction will be started within the next 6-months. Three visiting MSc-students will be coming from PPC (Bangkok, Thailand) to work on their MSc-projects (Sustainable process design of an olefin plant; Sustainability analysis of bioethanol production from rice straw; Development of a software tool for LCA) at CAPEC during July-September of this year.

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-batch and continuous process operations of biocatalytic reactions at miniature, lab and pilot scale is being developed. Both packed bed and stirred reactors are available. Analaytical equipment is in place.

HPLC analytical equipments for amino acid (right) and sugar(left)



HPLC analytical equipment for biodiesel

Packed bed reactor for transamination

Stirred tank reactor for enzymatic biodiesel production

Continuous stirred tank reactor for enzymatic biodiesel production

A pilot plant for enzymatic biodiesel production (reactor part)

A pilot plant for enzymatic biodiesel production (feeding tank part)

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. This course teaches the participants 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 (2010-2011)

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

	A - Ph.D. Theses and Monographs
PEC09-70	Rafiqul Gani, Henrique A. Matos and Ana Isabel Cerqueira de Sousa Gouveia Carvalho, 2010, "Sustainable Chemical Process Design", in "Managing CO2 Emissions in the Chemical Industry", Hans-Joachim Leimkuehler (Editor), Wiley-Vch, Germany, Chapter 5, pp. 159-188
PEC10-02 Book chp.	Rafiqul Gani, Vipasha Soni, Piotr T. Mitkowski, 2010, "Computer aided model based design and analysis of hybrid membrane reaction-separation systems", in "Comprehensive Membrane Science and Engineering", E. Drioli (Editor), Elsevier, The Netherlands
PEC10-13	Merlin Alvarado Morales, 2010, "Process-product synthesis, design and analysis through the Group Contribution (GC) approach", Ph.D. thesis
PEC10-23 Book chp.	Gunnar Jonsson and Francesca Macedonia, 2010, "Fundamentals in reverse osmosis", In "Comprehensive Membrane Science and Engineering", E. Drioli (Editor), Elsevier, The Netherlands, Vol. 2, pp. 1-21
PEC10-28	Elisa Conte, 2010, "Innovation in Integrated Chemical Product-Process Design - Development through a Model-based Systems Approach", Ph.D. thesis
PEC10-35	Oscar Andres Prado Rubio, 2010, "Integration of Bioreactor and Membrane Separation Processes: A Model Based Approach", Ph.D. thesis
PROCESS	Daniel Schäpper, 2010, "Continuous Culture Microbioreactors, Ph.D. thesis
PROCESS	Nanna Petersen Rønnest, 2010, "Analysis of Multivariate Sensor Data for Monitoring of Cultivations", Ph.D. thesis
PROCESS	Muhd. Nazrul Hisham Zainal Alam, **2011**, "Continuous Membrane Microbioreactor for Development of Integrated Pectin Modification and Separation Processes", Ph.D. thesis
PEC11-02	Mohd. Kamaruddin bin Abd. Hamid, **2011**, "Model-Based Integrated Process Design and Controller Design of Chemical Processes", Ph.D. thesis
PEC11-03	Rasmus Wedberg, **2011**, "Molecular Modeling of Enzyme Dynamics Towards Understanding Solvent Effects", Ph.D. thesis
PEC11-13	Martin D. Ellegaard, **2011**, "Molecular thermodynamics using fluctuation solution theory", Ph.D. thesis
PROCESS	Bodil Voss, **2011**, "Value-added Chemicals from Biomass by Heterogeneous Catalysis", Ph.D. thesis

PEC11-14	Ricardo Morales-Rodriguez, Rafiqul Gani, Stéphane Déchelotte, Alain Vacher and Olivier Baudouin, 2011, "Interoperability between Modelling Tools (MoT) with Thermodynamic Property Prediction Packages (Simulis® Thermodynamics) and Process Simulators (ProSimPlus) Via CAPE-OPEN Standards" in "Thermodynamics", ISBN: 978-953-307-544-0, Volume 1, Chapter 20, pp. 425-440

	B - Reviewed publications in International Journals
PEC08-29	Søren Prip Beier, Gunnar Jonsson, 2010, "Critical flux determination by flux-stepping", AIChE Journal, 56(7), pp. 1739-1747
PEC08-32	Roberta Ceriani, Antonio J.A. Meirelles, Rafiqul Gani, 2010, "Simulation of thin-film deodorizers in palm oil refining", Journal of Food Process Engineering, 33, pp. 208-225
PEC09-02	Netta Liin Rossing, Morten Lind, Niels Jensen and Sten Bay Jørgensen, 2010, "A Functional HAZOP Methodology", Computers and Chemical Engineering, 34(2), pp. 244–253
PEC09-06	R. Singh, K.V. Gernaey, R. Gani, 2010, "ICAS-PAT: A Software for Design, Analysis and Validation of PAT Systems", Computers & Chemical Engineering, 34(7), 1108-1136
PEC09-10	Kavitha C. Satyanarayana, Jens Abildskov, Rafiqul Gani, Georgia Tsolou, Vlasis G. Mavrantzas, 2010, "Computer aided polymer design using multiscale modeling**",** Brazilian Journal of Chemical Engineering, 27, 369-380
PEC09-31	M.V. Ruano, J. Ribes, Gürkan Sin, A. Seco and J. Ferrer, 2010, "A systematic approach for fine-tuning of fuzzy controllers applied to WWTPs", Environmental Modelling and Software, 25(5), 670-676
PEC09-48	Gürkan Sin, Anne S. Meyer and Krist V. Gernaey, 2010, "Assessing Reliability of Cellulose Hydrolysis Models to Support Biofuel Process Design – Identifiability and Uncertainty Analysis", Computers and Chemical Engineering 34, 1385–1392
PEC09-49	Jose Seoane, Gürkan Sin, Laurent Lardon, Krist V. Gernaey, Barth F. Smets, 2010, "A new extant respirometric assay to estimate intrinsic growth parameters applied to study plasmid metabolic burden", Biotechnology and Bioengineering, 105(1), 141–149
PEC09-52	Oscar Andres Prado-Rubio, Martin Møllerhøj, Sten B. Jørgensen, Gunnar E. Jonsson, 2010, "Modeling Donnan Dialysis Separation for Carboxylic Anion Recovery", Computers and Chemical Engineering, 34, 1567-1579
PEC09-53	Mohd Kamaruddin Abd Hamid; Gurkan Sin; Rafiqul Gani, 2010, "Integration of process design and controller design for chemical processes using model-based methodology", Computers and Chemical Engineering, 34(5), 683-699
PEC09-54	Wedberg R., Peters G.H., O'Connell J.P., Abildskov J., 2010, "Accurate Kirkwood–Buff integrals from molecular simulations", Molecular Simulation, 36(15), 1243-1252
PEC09-55	Naveed Ramzan, Muhammad Faheem, Rafiqul Gani, Werner Witt, 2010, "Multiple Steady States Detection in a Packed-Bed Reactive Distillation Column using Bifurcation Analysis", Computers & Chemical Engineering, 34(4), 460-466

PEC09-61	Krist V. Gernaey, Anna Eliasson Lantz, Pär Tufvesson, John M. Woodley and Gürkan Sin, 2010, "Application of mechanistic models to fermentation and biocatalysis for next-generation processes", Trends in Biotechnology, 28(7), 346-354
PEC09-65	Carlos A. Diaz-Tovar, Roberta Ceriani, Rafiqul Gani and Bent Sarup, 2010, "Systematic methodology and property prediction of fatty systems for process design/analysis in the oil and fat industry**",** Brazilian Journal of Chemical Engineering, 27, 401-412
PEC09-66	Merlin Alvarado–Morales, Mohd. Kamaruddin Abd Hamid, Gürkan Sin, Krist V. Gernaey, John M. Woodley and Rafiqul Gani, 2010, "A Model-Based Methodology for Simultaneous Design and Control of a Bioethanol Production Process", Computers and Chemical Engineering Journal, 34(12), 2043-2061
PEC09-67	Romain Privat, Rafiqul Gani and Jean-Noël Jaubert, 2010, "Are safe results obtained when the PC-SAFT equation of state is applied to ordinary chemicals?", Fluid Phase Equilibria, 295, 76-95
PEC09-68	Veronique van Speybroeck, Rafiqul Gani and Robert Johan Meier, 2010, "The calculation of thermodynamic properties of molecules", Chemical Society Review, 39(5), 1764-1779
PEC09-71	Ravendra Singh, Krist V. Gernaey, Rafiqul Gani, 2010, "An ontological knowledge based system for selection of process monitoring and analysis tools", Computers and Chemical Engineering, 34(7), 1137-1154
PEC09-74	Jakob Kjøbsted Huusom, Niels Kjølstad Poulsen and Sten Bay Jørgensen, 2010, "Iterative Feedback Tuning of Uncertain State Space Systems", Brazilian Journal of Chemical Engineering, 27(3), 461-472
PEC09-78	Manuel Pinelo, Gunnar Jonsson, Anne S. Meyer, 2009, "Membrane technology for purification of enzymatically produced oligosaccharides: Molecular and operational features affecting performance", Separation and Purification Technology, 70(1), 1-11
PEC10-03	Bao Lin, Sten Bay Jørgensen, **2011**, "Soft sensor design by multivariate fusion of image features and process measurements", Journal of Process Control, doi: 10.1016/j.jprocont.2011.01.006
PEC10-04	Abildskov J., Ellegaard M.D., O'Connell J.P., 2010, "Densities and isothermal compressibilities of ionic liquids - Modelling and application", Fluid Phase Equilibria, 295, 215-229
PEC10-05	Martin D. Ellegaard, Jens Abildskov, John P. O'Connell, 2010, "Molecular Thermodynamic Modelling of Mixed Solvent Solubility", Industrial & Engineering Chemistry Research, 49, 11620-11632
PEC10-08	Gürkan Sin, Krist V. Gernaey, Marc B. Neumann, Mark C.M. van Loosdrecht and Willi Gujer, **2011**, "Global sensitivity analysis in wastewater treatment plant model applications: Prioritizing sources of uncertainty", Water Research, 45(2), 639-651
PEC10-10	R. Ganigué, E.I.P. Volcke, S. Puig, M.D. Balaguer, J. Colprim and G. Sin, 2010, "Systematic model development for partial nitrification of landfill leachate in a SBR", Biotechnology and Bioengineering, 61(9), 2199-2210
PEC10-14	K.V. Gernaey, R. Gani, 2010, "A Model-based Systems Approach to Pharmaceutical Product-Process Design and Analysis", Chemical Engineering Science, 65(21), 5757-5769

PEC10-15	A.Carvalho, H.A. Matos, R. Gani, 2009, "Design of batch operations: Systematic methodology for generation and analysis of sustainable alternatives", Computers and Chemical Engineering, 33(12), 2075-2090
PEC10-16	C.A. Diaz Tovar, R. Gani, B. Sarup, **2011**, "Lipid technology: Property prediction and process design/analysis in the edible oil industries", Fluid Phase Equilibria, 302, 284-293
PEC10-18	A.A. Mustaffa, G.M. Kontogeorgis, R. Gani, **2011**, "Analysis and application of GC plus models for property prediction of organic chemical systems", Fluid Phase Equilibria, 302, 274-283
PEC10-19	Elisa Conte, Rafiqul Gani and Tahir I. Malik, **2011**, "The virtual product-process design laboratory to manage the complexity in the verification of formulated products", Fluid Phase Equilibria, 302, 294-304
PEC10-20	P. Lutze, R. Gani, J.M. Woodley, 2010, "Process Intensification: A Perspective on Process Synthesis", Chemical Engineering and Processing: Process Intensification, 49, 547-558
PEC10-21	P. Lutze, E. Dada, R. Gani, J.M. Woodley, 2010, "Heterogeneous Catalytic Distillation - A Patent Review", Recent Patents on Chemical Engineering, 3, (e-journal)
PEC10-22	Morales Rodriguez, Ricardo; Gernaey, Krist; Meyer, Anne S.; Sin, Gürkan, **2011**, "A Mathematical Model for Simultaneous Saccharification and Co-fermentation (SSCF) of C6 and C5 Sugars", Chinese Journal of Chemical Engineering 19(2), pp. 185-191
PEC10-27	Martin D. Ellegaard, Jens Abildskov, John P. O'Connell, **2011**, "Solubilities of gases in ionic liquids using a corresponding-states approach to Kirkwood-Buff solution theory", Fluid Phase Equilibria, Special Issue PPEPPD 2010, 302, 93-102
PEC10-29	Corominas L., Sin G., Puig S., Balaguer M.D., Vanrolleghem P.A., Colprim J., **2011**, "Modified calibration protocol evaluated in a model-based testing of SBR flexibility", Bioprocess and Biosystems Engineering, 34, 205-214
PEC10-30	Rasmus Wedberg, John P. O'Connell, Günther H. Peters, Jens Abildskov, **2011**, "Total and Direct Correlation Function Integrals from Molecular Simulation of Binary Systems", Fluid Phase Equilibria, 302(1-2), 32-42
PEC10-31	Prado-Rubio, O.A.; Jørgensen, S.B. and Jonsson, G., **2011**, "Model based investigation of the potential lactate recovery using Electro-Enhanced Dialysis - Static analysis", Separation and Purification Technology Journal, 78, 113-124
PEC10-32	Prado-Rubio, O.A.; Jørgensen, S.B. and Jonsson, G., **2011**, "Reverse Electro-Enhanced Dialysis for lactate recovery from a fermentation broth", Journal of Membrane Science, 374(1-2), 20–32
PEC10-33	Ricardo Morales-Rodriguez, Anne S. Meyer, Krist V. Gernaey, Gürkan Sin, **2011**, "Dynamic Model-Based Evaluation of Process Configurations for Integrated Operation of Hydrolysis and Co-Fermentation for Bioethanol Production from Lignocellulose", Bioresource Technology Journal, 102(2), 1174-1184
PEC10-34	Conte E., Gani R. and Ng K. M., **2011**, "Design of formulated products: a systematic methodology", AIChE Journal, DOI: 10.1002/aic.12458

PEC10-37	Abildskov J., Ellegaard M.D., O'Connell J.P., 2010, "Phase Behavior of Mixtures of Ionic Liquids and Organic Solvents", Journal of Supercritical Fluids (100th year Anniversary of van der Waals' Nobel Lecture), 55, 833–845
PEC10-38	Abdul Samad, Noor Asma Fazli; Singh, Ravendra; Sin, Gürkan; Gernaey, Krist; Gani, Rafiqul, **2011**, "A generic multi-dimensional model-based system for batch cooling crystallization processes", Computers & Chemical Engineering, 35 (5),828-843 (doi:10.1016/j.compchemeng.2011.01.029)
PEC10-39	Netta Liin Rossing, Morten Lind, Niels Jensen, Sten B. Jørgensen, 2010, "A Goal based methodology for HAZOP analysis", International Journal of Nuclear Safety and Simulation, 1, 134-142
PEC10-41	Heitzig, Martina; Sin, Gurkan; Sales Cruz, Mauricio; Glarborg, Peter; Gani, Rafiqul, **2011**, "A computer-aided modeling framework for efficient model development, analysis and identification: Combustion and reactor modeling", Industrial & Engineering Chemistry Research Puigjaner Special Issue, 50, 5253-5265 (DOI: 10.1021/ie101393q)
PEC10-43	E. Conte, R. Gani, Y. S. Cheng, K. M. Ng, **2011**, "Design of Formulated Products: Experimental Component", AIChE Journal, DOI 10.1002/aic.12582
PEC10-48	E. Zondervan, Mehboob Nawaz, André B de Haan, John M Woodley, Rafiqul Gani, **2011**, "Optimal design of a multi-product biorefinery system", Computers and Chemical Engineering Journal (Special Issue: Energy Systems Engineering), doi:10.1016/j.compchemeng.2011.01.042
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	F - Conference Presentations 2010
2010-1	Ana Carvalho, Rafiqul Gani and Henrique Matos , 2010, "Design of sustainable processes: Systematic generation and evaluation of alternatives", 2nd Annual Gas Processing Symposium 2010, Doha, Qatar, 11-14 January **(Best Paper Award)**
2010-2	Rafiqul Gani, 2010, "Design challenges and sustainability issues in gas processing: A view from academia", 2nd Annual Gas Processing Symposium 2010, Doha, Qatar, 11-14 January **(Invited Lecture)**
2010-3	Gürkan Sin, Anna Eliasson Lantz, Krist V. Gernaey, 2010, "Perspectives on the use of global uncertainty and sensitivity analysis methods in a PAT context", 24th International Foundation Process Analytical Chemistry (IFPAC®), Baltimore, Maryland, USA, 31 January – 4 February
2010-4	Ravendra Singh, Noor Asma Fazli Abdul Samad, Krist V. Gernaey, John M. Woodley, Rafiqul Gani, 2010, "Mechanistic modeling for systematic design and analysis of PAT systems", 24th International Foundation Process Analytical Chemistry (IFPAC®), Baltimore, Maryland, USA, 31 January - 4 February **(Invited Lecture)**
(poster) 2010-5	Carlos Axel Díaz-Tovar, Rafiqul Gani, Bent Sarup, 2010, "Towards the Merging of Property Prediction & Process Design/Analysis in the Edible Oil Industry", CAPE Forum 2010, Aachen, Germany, 11-12 March
2010-6	Jakob Kjøbsted Huusom, Niels Kjølstad Poulsen, Sten Bay Jørgensen, John Bagterp Jørgensen, 2010, "Tuning of ARX-based Model Predictive Control for Offset-free Tracking", CAPE Forum, Aachen, Germany, 11-12 March
2010-7	Mohd. Kamaruddin Abd. Hamid, Gurkan Sin, Rafiqul Gani, 2010, "Application of Decomposition Methodology to Solve Integrated Process Design and Controller Design Problems for Reactor-Separator-Recycle Systems", CAPE Forum, Aachen, Germany, 11-12 March
2010-8	Alicia Román-Martínez, Rafiqul Gani, John M. Woodley, 2010, "Model-based Design and Analysis of Integrated Biocatalytic Processes", CAPE Forum 2010, Aachen, Germany, 11-12 March
2010-9	Rafiqul Gani, 2010, "Thermodynamics – our molecular sister or just a forgotten relative?", CAPE Forum 2010, Aachen, Germany, 11-12 March **(Invited Lecture)**
2010-10	Gürkan Sin, M.V. Ruano, Marc B. Neumann, J. Ribes, Krist V. Gernaey, J. Ferrer , Mark C.M. van Loosdrecht and Willi Gujer, 2010, "Sensitivity analysis in the WWTP modelling community – new opportunities and applications", 2nd IWA/WEF Wastewater Treatment Modelling Seminar, Mont-Sainte-Anne, Quebec, Canada. March 26-31
2010-11	Sascha Sansonetti, Stefano Curcio, Vincenza Calabrò, Gürkan Sin and Gabriele Iorio, 2010, "Feasibility of the batch fermentation process of Ricotta Cheese Whey (RCW)", IBIC2010, Padua, Italy, 11-14 April
2010-12	Singh, R., Samad, N.A.F.A., Sin, G., Gernaey, K. V., Gani, R., 2010, "Systematic method and tool for design, analysis &/or validation of PAT systems", APACT-10, Manchester, UK, 28-30 April

(poster) 2010-13	Fu, W., Jensen, J. S., Boisen, A., Pedersen, S., Riisager, A., Gani, R., Woodley, J., 2010, "Process Design for Chemo-enzymatic Synthesis of 2,5-Furandicarboxylic Acid", 2nd International Symposium on Sustainable Chemical Product and Process Engineering (2nd SCPPE), Hangzhou, China, 9-12 May **(Best Poster Award)**
Oral 2010-14	Fu, W., Jensen, J. S., Boisen, A., Pedersen, S., Riisager, A., Gani, R., Woodley, J., 2010, "Process Design for Chemo-enzymatic Synthesis of 2,5-Furandicarboxylic Acid", 2nd International Symposium on Sustainable Chemical Product and Process Engineering (2nd SCPPE), Hangzhou, China, 9-12 May
(poster) 2010-15	N. Iyara, K. Siemanond, R. Gani, 2010, "Sustainable design for an olefin process", 2nd International Symposium on Sustainable Chemical Product and Process Engineering (2nd SCPPE), Hangzhou, China, 9-12 May **(Best Poster Award)**
(poster) 2010-16	P. Tansutapanich, P. Malakul, R. Gani, 2010, "Sustainable process design for lignocellulosic-based bioethanol using life cycle assessment technique", 2nd International Symposium on Sustainable Chemical Product and Process Engineering (2nd SCPPE), Hangzhou, China, 9-12 May
2010-17	R. Gani, 2010, "Solvents, green chemistry and sustainable product-process design", 2nd International Symposium on Sustainable Chemical Product and Process Engineering (2nd SCPPE), Hangzhou, China, 9-12 May **(Plenary Lecture)**
2010-18	Ricardo Morales-Rodriguez, Krist V. Gernaey, Anne S. Meyer and Gürkan Sin, 2010, "Development of a mathematical model describing hydrolysis and co-fermentation of C6 and C5 sugars", 2nd International Symposium on Sustainable Chemical Product and Process Engineering (2nd SCPPE), Hangzhou, China, 9-12 May
(poster) 2010-19	C.A. Diaz Tovar, R. Gani, B. Sarup, 2010, "Lipid technology: Property prediction and process design/analysis in the edible oil industry", PPEPPD-2010, Suzhou, Jiangsu, China, 16-21 May
(poster) 2010-20	C. Aguirre, L. Cisternas, J. Continho, R. Gani, 2010, "Computer-aided design of ionic-liquids by group contribution methods", PPEPPD-2010, Suzhou, Jiangsu, China, 16-21 May
(poster) 2010-21	A.A. Mustaffa, G.M. Kontogeorgis, R. Gani, 2010, "Analysis and application of GC plus models for property prediction of organic chemical systems", PPEPPD-2010, Suzhou, Jiangsu, China, 16-21 May
2010-22	Elisa Conte, Rafiqul Gani and Tahir I. Malik, 2010, "The Virtual Product-Process Design Laboratory to Manage the Complexity in Formulation Design", PPEPPD-2010, Suzhou, Jiangsu, China, 16-21 May
2010-23	Ravendra Singh, Gürkan Sin, John M. Woodley, Krist V. Gernaey and Rafiqul Gani, 2010, "Methods and tools for systematic development of QbD.based pharmaceutical processes", BioProcess, Vienna, Austria, 19-20 May - withdrawn
(poster) 2010-24	Ricardo Morales-Rodriguez, Krist V. Gernaey, Anne S. Meyer, Gürkan Sin, 2010, "Integrated Dynamic Plant-Wide Model-Based Simulation of Bioethanol Production from Lignocellulose", Biokemisk Forening, Vejle, Denmark, 27–28 May
2010-25	Jakob Kjøbsted Huusom, Niels Kjølstad Poulsen, Sten Bay Jørgensen, John Bagterp Jørgensen, 2010, "ARX-Model based Model Predictive Control with Offset-Free Tracking", ESCAPE20, Ischia, Naples, Italy, 6-9 June

2010-26	Ricardo Morales-Rodriguez, Marie Capron, Jakob Kjøbsted Huusom and Gürkan Sin, 2010, ”Controlled fed-batch operation for enzymatic cellulose hydrolysis in 2G bioethanol production”, ESCAPE20, Ischia, Naples, Italy, 6-9 June
2010-27	Oscar Andres Prado-Rubio, Sten Bay Jørgensen and Gunnar Jonsson, 2010, ”Control System Development for Integrated Bioreactor and Membrane Separation Process”, ESCAPE20, Ischia, Naples, Italy, 6-9 June
2010-28	Oscar Andres Prado-Rubio, John Bagterp Jørgensen and Sten Bay Jørgensen, 2010, ”Systematic Model Analysis for Single Cell Protein (SCP) Production in a U-Loop Reactor”, ESCAPE20, Ischia, Naples, Italy, 6-9 June
(poster) 2010-29	Merlin Alvarado-Morales, Krist V. Gernaey, John M. Woodley, Rafiqul Gani, 2010, “Synthesis, Design and Analysis of Downstream Separation in Bio-refinery Processes through a Group-Contribution Approach”, ESCAPE20, Ischia, Naples, Italy, 6-9 June
2010-30	Philip Lutze, Alicia Román-Martinez, John M. Woodley, Rafiqul Gani, 2010, “A systematic synthesis and design methodology to achieve process intensification in (bio) chemical processes”, ESCAPE20, Ischia, Naples, Italy, 6-9 June
2010-31	Martina Heitzig, Gürkan Sin, Peter Glarborg, Rafiqul Gani, 2010, ”A computer-aided framework for regression and multi-scale-modelling needs in innovative product-process engineering”, ESCAPE20, Ischia, Naples, Italy, 6-9 June
2010-32	Elisa Conte, Rafiqul Gani, Tom Malik, 2010, “The Virtual Product-Process Laboratory applied to personal care formulations”, ESCAPE20, Ischia, Naples, Italy, 6-9 June
2010-33	Noor Asma Fazli Abdul Samad, Ravendra Singh, Gürkan Sin, Krist V. Gernaey, Rafiqul Gani, 2010, ”Control of Process Operations and Monitoring of Product Qualities through Generic Model-based in Batch Cooling Crystallization”, ESCAPE20, Ischia, Naples, Italy, 6-9 June
2010-34	Paloma A. Santacoloma, Gürkan Sin, Krist V. Gernaey and John M. Woodley, 2010, “Sensitivity Analysis of a Kinetic Model Describing the Bi-enzymatic Synthesis of Lactobionic Acid”, ESCAPE20, Ischia, Naples, Italy, 6-9 June
2010-35	Ravendra Singh, 2010, “Model-based computer-aided framework for design of process monitoring and analysis systems (PAT systems)”, Invited lecture, on the ceremony of EFCE Excellence Award for the Outstanding PhD Thesis on CAPE, from European Federation of Chemical Engineering (EFCE), ESCAPE20, Ischia, Naples, Italy, 6-9 June **(Invited Lecture + PhD Thesis Award)**
(poster) 2010-36	Rasmus Wedberg, Günther H. Peters, Jens Abildskov, 2010, “Studying Candida Antarctica Lipase B in Organic Solvents at Fixed Water Activities using Molecular Dynamics Simulations”, IBBI 2010 (Isolated biomolecules and biomolecular interactions), Berlin, Germany, 12-17 June
(poster) 2010-37	Dawid Jan Bialas, Jakob Kjøbsted Huusom John Bagterp Jørgensen, Gürkan Sin, 2010, “Model predictive control for reactor-separator-recycle system”, Dansk Kemiingeniørkonference - DK2-2010, Lyngby, Denmark, 16-17 June
(poster) 2010-38	Albert E. Cervera, Krist V. Gernaey, Rafiqul Gani, Søren Kiil and Tommy Skovby, 2010, “Moving from batch toward continuous organic-chemical pharmaceutical production”, Dansk Kemiingeniørkonference - DK2-2010, Lyngby, Denmark, 16-17 June

(poster) 2010-39	Elisa Conte and Rafiqul Gani 2010, "Formulation design: managing the complexity through the Virtual Laboratory", Dansk Kemiingeniørkonference - DK2-2010, Lyngby, Denmark, 16-17 June
(poster) 2010-40	Carlos A. Diaz-Tovar, Rafiqul Gani and Bent Sarup, 2010, "Lipid Technology: Merging Property Prediction & process Design/Analysis in the Edible Oil Industry", Dansk Kemiingeniørkonference - DK2-2010, Lyngby, Denmark, 16-17 June
(poster) 2010-41	Martin D. Ellegaard, Jens Abildskov and John P. O'Connell, 2010, "Modelling af opløseligheder i systemer med blandede solventer", Dansk Kemiingeniørkonference - DK2-2010, Lyngby, Denmark, 16-17 June
(poster) PROCESS	Rita Lencastre Fernandes, Daniel Schäpper, Fridolin Okkels, Anna Eliasson Lantz, Henrik Bruus, Krist V. Gernaey, 2010, "Structurally optimized microbioreactors for immobilized yeast cultivations", Dansk Kemiingeniørkonference - DK2-2010, Lyngby, Denmark, 16-17 June
(poster) 2010-42	Wenjing Fu, Astrid Boisen, Sven Pedersen, Rafiqul Gani, John Woodley, Jacob S. Jensen, Anders Riisager, 2010, "Process Design for Chemo-enzymatic Synthesis of 5-Hydroxymethylfurfural", Dansk Kemiingeniørkonference - DK2-2010, Lyngby, Denmark, 16-17 June
(poster) 2010-43	Mohd. Kamaruddin Abd. Hamid, Gürkan Sin and Rafiqul Gani, 2010, "Application of Decomposition Methodology to Solve Integrated Process Design and Controller Design Problem for Reactor-Separator-Recycle System", Dansk Kemiingeniørkonference - DK2-2010, Lyngby, Denmark, 16-17 June
(poster) 2010-44	Martina Heitzig, Gürkan Sin, Peter Glarborg and Rafiqul Gani, 2010, "Computer-Aided Modelling for Efficient and Innovative Product-Process Engineering", Dansk Kemiingeniørkonference - DK2-2010, Lyngby, Denmark, 16-17 June
(poster) 2010-45	Jakob Kjøbsted Huusom, Niels Kjølstad Poulsen, Sten Bay Jørgensen and John Bagterp Jørgensen, 2010, "Tuning of ARX-based Model Predictive Control for Offset-free Tracking", Dansk Kemiingeniørkonference - DK2-2010, Lyngby, Denmark, 16-17 June
(poster) 2010-46	Philip Lutze, Rafiqul Gani, John M. Woodley, 2010, "Development of a Systematic Synthesis/Design Methodology incorporating Process Intensification", Dansk Kemiingeniørkonference - DK2-2010, Lyngby, Denmark, 16-17 June
(poster) PROCESS	Tine Kranker, Lene Svendsen, Rita Lencastre Fernandes and Krist V. Gernaey, 2010, "A Population Balance Model for Microbial Populations in Fermentors", Dansk Kemiingeniørkonference - DK2-2010, Lyngby, Denmark, 16-17 June
(poster) 2010-47	Ricardo Morales-Rodriguez, Krist V. Gernaey, Anne Meyer, Gürkan Sin, 2010, "Integrated Dynamic Plant-Wide Model-Based Simulation of Bioethanol Production from Lignocellulose", Dansk Kemiingeniørkonference - DK2-2010, Lyngby, Denmark, 16-17 June
(poster) PROCESS	Mathias Nordblad, Yuan Xu, Lars Saaby Pedersen, John M. Woodley, 2010, "Impact of reaction engineering parameters on process design for enzyme-based FAEE-biodiesel production", Dansk Kemiingeniørkonference - DK2-2010, Lyngby, Denmark, 16-17 June
(poster) 2010-48	Alicia Román-Martínez, Rafiqul Gani, John M. Woodley, 2010, "Model-based design and analysis of integrated biocatalytic processes", Dansk Kemiingeniørkonference - DK2-2010, Lyngby, Denmark, 16-17 June

(poster) PROCESS	Nanna Petersen Rønnest, Stuart Stocks, Anna Eliasson Lantz, Krist V. Gernaey, 2010, "Sammenligning af avancerede online sensorer til måling af biomassekoncentrationen i filamentøse fermenteringer", Dansk Kemiingeniørkonference - DK2-2010, Lyngby, Denmark, 16-17 June
(poster) PROCESS	Paloma A. Santacoloma, Gürkan Sin, Krist V. Gernaey and John M. Woodley, 2010, "New concepts for multi-enzymatic synthetic processes", Dansk Kemiingeniørkonference - DK2-2010, Lyngby, Denmark, 16-17 June
(poster) PROCESS	Peter N.R. Vennestrøm, Sven Pedersen, Claus H. Christensen, Jan-Dierk Grunwaldt, John M. Woodley, 2010, "Combining enzymes with heterogeneous chemical catalysts: chemoenzymatic combination of oxidase enzymes with titanium silicalite-1", Dansk Kemiingeniørkonference - DK2-2010, Lyngby, Denmark, 16-17 June
(poster) PROCESS	Tindal, S.R., Xue, R., Archer, I.V.J., Carr, R., Farid, S., Hailes, H.C., & Woodley, J.M., 2010, "Enzymatic Bioprocess Considerations when Changing Substrate", Dansk Kemiingeniørkonference - DK2-2010, Lyngby, Denmark, 16-17 June
(poster) 2010-49	Linfeng Yuan, Gunnar Jonsson, John Woodley, Lars Korsholm, 2010, "Electro-membrane filtration for amino acid separation", Dansk Kemiingeniørkonference - DK2-2010, Lyngby, Denmark, 16-17 June
2010-50	Jens Ulrik Rype, Arvid Garde and Gunnar Jonsson, 2010, "Combining membrane separation technology and fermentation processes for improved performances", Dansk Kemiingeniørkonference - DK2-2010, Lyngby, Denmark, 16-17 June
2010-51	Gürkan Sin, 2010, "Uncertainty in modelling, design and operation of chemical processes", Dansk Kemiingeniørkonference - DK2-2010, Lyngby, Denmark, 16-17 June
PROCESS	Mads Orla Albaek, KV Gernaey, MS Hansen and SM Stocks, 2010, "Comparison of Traditional Rushton Disc Turbines with Up-pumping Hydrofoil B2 Impellers in 550 L Pilot Scale Aerobic Submerged Fermentations", Dansk Kemiingeniørkonference - DK2-2010, Lyngby, Denmark, 16-17 June
2010-52	Dres Foged Olsen, John Bagterp Jørgensen, John Villadsen, Sten Bay Jørgensen, 2010, "Single-Cell Protein Production in a U-Loop Reactor", Dansk Kemiingeniørkonference - DK2-2010, Lyngby, Denmark, 16-17 June
PROCESS	Bodil Voss, Jan-Dierk Grunwaldt, John Woodley and Simon Ivar Andersen, 2010, "Chemicals from Biomass: Sustainability and Feasibility of a Cu-based Catalyst", Dansk Kemiingeniørkonference - DK2-2010, Lyngby, Denmark, 16-17 June
PROCESS	A.H. Feyissa, J. Adler-Nissen and K.V. Gernaey, 2010, "Approaches to Robust Modelling of Frying Processes", Dansk Kemiingeniørkonference - DK2-2010, Lyngby, Denmark, 16-17 June
PROCESS	Krist V. Gernaey, Daniel Schäpper, Muhd Nazrul Hisham Zainal Alam, Andrijana Bolic, 2010, "Microreactors for Application in biotech Process Development", Dansk Kemiingeniørkonference - DK2-2010, Lyngby, Denmark, 16-17 June
2010-53	Rafiqul Gani, 2010, "Computer aided molecular and blend design applied to fuel-related products", 3rd TMFB International Workshop, RWTH Aachen, Germany, 23-24 June **(Invited Lecture)**

2010-54	Jakob Kjøbsted Huusom, Niels Kjølstad Poulsen, Sten Bay Jørgensen and John Bagterp Jørgensen, 2010, ”Tuning of Methods for Offset Free MPC based on ARX Model Representations”, American Control Conference (ACC), Baltimore, Maryland, USA, 30 June - 2 July
2010-55	Dres Foged Olsen; John Bagterp Jørgensen; John Villadsen.; Sten Bay Jørgensen, 2010, ”Modeling and Simulation of Single Cell Protein Production”, 11th Computer Applications in Biotechnology, CAB 2010, Leuven, Belgium, 5-7 July
2010-56	Dres Foged Olsen; John Bagterp Jørgensen; John Villadsen.; Sten Bay Jørgensen, 2010, ”Optimal Operating Points for SCP Production in the U-Loop Reactor”, 9th International Symposium on Dynamics and Control of Process Systems, DYCOPS 2010, Leuven, Belgium, 7-9 July
2010-57	Mohd. Kamaruddin Abd. Hamid, Gürkan Sin and Rafiqul Gani, 2010, ”Application of Decomposition Methodology to Solve Integrated Process Design and Controller Design Problems for Reactor-Separator-Recycle Systems”, 9th International Symposium on Dynamics and Control of Process Systems, DYCOPS 2010, Leuven, Belgium, 7-9 July
2010-58	Martina Heitzig, Gürkan Sin, Peter Glarborg, Rafiqul Gani, 2010, ”A Computer-Aided Framework for Systematic Model Development, Analysis, and Identification in Innovative Product-Process Engineering”, 6th International Conference on Sensitivity Analysis of Model Output, Milan, Italy, 19-22 July
2010-59	R. Gani, 2010, ”Property Modelling for Applications in Chemical Product and Process Design”, 21st IUPAC International Conference on Chemical Thermodynamics ICCT-2010, Tsukuba, Japan, 31 July – 6 August **(Invited Lecture)**
2010-60	C.A. Diaz-Tovar, R. Gani and B. Sarup, 2010, “Methods and Tools to Overcome the Lack of Data in Property Prediction in Lipid Processing Technology”, 21st IUPAC International Conference on Chemical Thermodynamics ICCT-2010, Tsukuba, Japan, 31 July – 6 August
2010-61	Dawid Jan Białas, Jakob Kjøbsted Huusom, John Bagterp Jørgensen, Gürkan Sin, 2010, “Model predictive control for plant-wide control of a reactor-separator-recycle system”, 16th Nordic Process Control Workshop – NPCW16, Lund, Sweden, 26-27 August
2010-62	Jakob Kjøbsted Huusom, Niels Kjølstad Poulsen, Sten Bay Jørgensen and John Bagterp Jørgensen, 2010, ”Tuning of ARX-based Model Predictive Control for Offset-free Tracking”, 16th Nordic Process Control Workshop - NPCW16, Lund, Sweden, 26-27 August
2010-63	Singh, R., Gernaey, K. V., Gani, R., 2010, “Systematic computer-aided method and tool (ICAS-PAT) for design, analysis &/or validation of process monitoring and analysis systems (PAT systems)”, CHISA2010/ECCE-7, Prague, Czech Republic, 28 August – 1 September
2010-64	F. Muller, R. R. Sanchez, T. Wrate, S. Davison, A. Manipura, E. B. Martin, G. A. Montague, M. Kraut, K. Haas-Santo, K. Forsberg, A. C. Rasmuson, R. Singh, K. V. Gernaey, R. Gani, J. M. Woodley, 2010, “F^3 process design for fine chemical and Pharmaceutical transformations”, CHISA2010/ECCE-7, Prague, Czech Republic, 28 August – 1 September

2010-65	R. Morales-Rodriguez, K.V. Gernaey, A.S. Meyer and G. Sin, 2010, ”Dynamic plant-wide modelling for bioethanol production from lignocellulosic biomass (2G)”, CHISA2010/ECCE-7, Prague, Czech Republic, 28 August - 1 September
2010-66	Martina Heitzig, Gürkan Sin, Peter Glarborg, Rafiqul Gani, 2010, ”A computer-aided modelling framework for use in product-process engineering”, CHISA2010/ECCE-7, Prague, Czech Republic, 28 August - 1 September
2010-67	Philip Lutze, Jacob Skibsted Jensen, Rafiqul Gani, John M. Woodley, 2010, “A systematic methodology to synthesize/design processes, incorporating process intensification”, CHISA2010/ECCE-7, Prague, Czech Republic, 28 August – 1 September
(poster) 2010-68	Philip Lutze, Jacob Skibsted Jensen, Rafiqul Gani, John M. Woodley, 2010, “A systematic synthesis and design methodology to achieve process intensification for multi-phase reactions”, CHISA2010/ECCE-7, Prague, Czech Republic, 28 August – 1 September
2010-69	Fu W., Jensen J.S., Riisager A., Gani R., Woodley J.M., Boisen A. and Pedersen S., 2010, “Process design for chemo-enzymatic synthesis of 5-hydroxymethylfurfural”, BEST 2010, Bologna, Italy, 5-8 September
(poster) 2010-70	Fu W., Jensen .J.S., Riisager A., Pedersen S., Gani R. and Woodley J.M., 2010, “Process design for chemo-enzymatic synthesis of 5-hydroxymethylfurfural”, BEST 2010, Bologna, Italy, 5-8 September
2010-71	Santacoloma P.A., Sin G., Gernaey K.V. and Woodley J.M., 2010, “New concepts for multi-enzymatic synthetic processes”, BEST 2010, Bologna, Italy, 5-8 September
(poster) 2010-72	Al-Haque N., Tufvesson P., Gani R. and Woodley J.M., 2010, “Application of Solid Resins for Controlled Substrate supply to biocatalytic reactions”, BEST 2010, Bologna, Italy, 5-8 September
(poster) 2010-73	Samad, N. A. F. A., Singh, R., Sin, G., Gernaey, K. V., Gani, R., 2010, “A Generic Model-Based Framework for Batch Cooling Crystallization Processes”, PBM2010 (4th International Conference on Population Balance Modeling), Berlin, Germany, 15–17 September
2010-74	George Sprouse, Jeff McCormick, Olivier Schraa and Gürkan Sin, 2010, ”IWA Design and Operational Uncertainty Task Group: Document and evaluate existing methods for assessing and evaluating uncertainty in wastewater treatment”, IWA World water congress and exhibition, Montreal, Canada, 19-24 September
2010-75	Rafiqul Gani, 2010, ”Solvents, green chemistry and sustainable product-process design”, Slovenian Chemical Technology Conference 2010, Ljubljana, Slovenia, 23 September **(Invited Plenary Lecture)**
2010-76	Ricardo Morales-Rodriguez, Anne Meyer, Krist V. Gernaey, Gürkan Sin, 2010, “From lab experiments to plant operation and design: Bioethanol production from lignocellulose using different enzyme technologies”, 2nd Annual workshop on enzymatic hydrolysis of insoluble substrates, Holbæk, Denmark, 26-27 October
2010-77	Anna Katrine Vangsgaard, Gürkan Sin, Krist V. Gernaey and Barth F. Smets, 2010, ”Validation of Structured Model of Complete Autotrophic Nitrogen Removal”, Research center EcoDesign-MBR meeting, Aalborg, Denmark, 5 November

2010-78	Lutze, Philip; Gani, Rafiqul; Woodley, John M.; Dada, Emmanuel A., 2010, "Recent Advances in Reactive Distillation", NOBCChE (National Organization of Black Chemists and Chemical Engineers) Conference, University of Pennsylvania, Philadelphia, USA, 5-6 November
PROCESS	Nanna Petersen, Stuart M. Stocks, Anna Eliasson Lantz and Krist V. Gernaey, 2010, "Biomass Measurements in Filamentous Fermentations: Comparison of Advanced On-Line Sensors", AIChE Annual Meeting, Salt Lake City, Utah, USA, 7-12 November
2010-79	Roman Martinez A., Gani R. and Woodley J.M., 2010, "Implementation of Novel Integrated Pharmaceutical Processes: A Model-based Approach", AIChE Annual Meeting, Salt Lake City, Utah, USA, 7-12 November
2010-80	Martina Heitzig, Gürkan Sin, Peter Glarborg, Rafiqul Gani, 2010, "Managing Multi-Scale Modeling Issues in Chemical Engineering – a Computer-Aided Framework", AIChE Annual Meeting, Salt Lake City, Utah, USA, 7-12 November
2010-81	Noor Asma Fazli Abdul Samad, Ravendra Singh, Gürkan Sin, Krist Gernaey and Rafiqul Gani, 2010, "A Generic Multi-Dimensional Model-Based Framework for Batch Cooling Crystallization Process", AIChE Annual Meeting, Salt Lake City, Utah, USA, 7-12 November
2010-82	Ricardo Morales-Rodríguez, Anne S. Meyer, Krist V. Gernaey and Gürkan Sin, 2010, "Process Technology Evaluation for Lignocellulosic Bioethanol Production: Plantwide Configurations Using a Dynamic Modeling Approach", AIChE Annual Meeting, Salt Lake City, Utah, USA, 7-12 November
2010-83	Carlos Axel Diaz-Tovar, Rafiqul Gani and Bent Sarup, 2010, "Property Prediction for Lipids Based Product Design and Analysis", AIChE Annual Meeting, Salt Lake City, Utah, USA, 7-12 November
2010-84	Elisa Conte and Rafiqul Gani, 2010, "Managing the Complexity in Liquid Formulation Design", AIChE Annual Meeting, Salt Lake City, Utah, USA, 7-12 November
2010-85	Philip Lutze, Rafiqul Gani, John M. Woodley, 2010, "Application of a Synthesis and Design Methodology Incorporating Process Intensification", AIChE Annual Meeting, Salt Lake City, Utah, USA, 7-12 November
2010-86	Singh R., Gernaey K.V., Gani R. and Woodley J.M., 2010, "Systematic Framework for Design and Adaption of Fast, Flexible, Continuous Modular Plants", AIChE Annual Meeting, Salt Lake City, Utah, USA, 7-12 November
2010-87	Albert E. Cervera, Krist V. Gernaey, Rafiqul Gani, Søren Kiil and Tommy Skovby, 2010, "Design of Continuous Processes for Organic-Synthesis Based Production of Active Pharmaceutical Ingredients – a Methodology",AIChE Annual Meeting, Salt Lake City, Utah, USA, 7-12 November
2010-88	Philip Lutze, Rafiqul Gani, John M. Woodley and Emmanuel A. Dada, 2010, "Recent Advances in Reactive Distillation", AIChE Annual Meeting, Salt Lake City, Utah, USA, 7-12 November
2010-89	Ravendra Singh, Krist V. Gernaey, Gani Rafiqul and John M. Woodley, 2010, "An Ontological Knowledge-Based System for Identification of Efficient Chemical Production Routes", AIChE Annual Meeting, Salt Lake City, Utah, USA, 7-12 November

2010-90	Martina Heitzig, Gürkan Sin, Peter Glarborg, Rafiqul Gani, 2010, "ICAS-MoT, a Computer-Aided Modeling Tool", AIChE Annual Meeting, Salt Lake City, Utah, USA, 7-12 November
2010-91	Jonas Eeclo, Chien-Tai Tsai, Ricardo Morales-Rodríguez, Krist V. Gernaey, Anne S. Meyer and Gürkan Sin, 2010, "A Dynamic Model for Cellulosic Biomass Hydrolysis: Validation of Hydrolysis and Product Inhibition Mechanism", AIChE Annual Meeting, Salt Lake City, Utah, USA, 7-12 November
2010-92	Romain Privat, Jean-Noel Jaubert and Rafiqul Gani, 2010, "Are Safe Results Obtained When the PC-SAFT Equation of State Is Applied to Ordinary Pure Chemicals?", AIChE Annual Meeting, Salt Lake City, Utah, USA, 7-12 November
PROCESS	Krist V. Gernaey, Pär Tufvesson and John M. Woodley, 2010, "Process Development and Design for Greener Pharmaceutical Processes", AIChE Annual Meeting, Salt Lake City, Utah, USA, 7-12 November
2010-93	Muhd. Nazrul Hisham Zainal Alam, Manuel Pinelo, Anne S. Meyer, Gunnar E. Jonsson and Krist V. Gernaey, 2010, "Membrane Microbioreactor for Enzyme-Catalyzed Degradation of Pectin", AIChE Annual Meeting, Salt Lake City, Utah, USA, 7-12 November
PROCESS	Rita L. Fernandes, Daniel Schäpper, Fridolin Okkels, Anna Eliasson Lantz, Henrik Bruus and Krist V. Gernaey, 2010, "Structurally Optimized Microbioreactors: A Design Example for Immobilized Yeast Cultivations", AIChE Annual Meeting, Salt Lake City, Utah, USA, 7-12 November
(poster) 2010-94	Deenesh Babi, Jason Price and Rafiqul Gani, 2010, "Systematic Design of An Acetaldehyde Process", AIChE Annual Meeting, Salt Lake City, Utah, USA, 7-12 November
(poster) 2010-95	Jakob Kjøbsted Huusom, Niels Kjølstad Poulsen, Sten B. Jørgensen and John Bagterp Jørgensen, 2010, "ARX-based Model Predictive Control of Systems with Time Delays", AIChE Annual Meeting, Salt Lake City, Utah, USA, 7-12 November
2010-96	Lutze, Philip; Gani, Rafiqul; Woodley, John M.; Dada, Emmanuel A., 2010, "Recent Advances in Reactive Distillation", NSChE (Nigerian Society of Chemical Engineers), 40th Annual International Conference, Port Harcourt, Nigeria,18-20 November
	F - Conference Presentations 2011
2011-1	Nor Alafiza Yunus, Krist V. Gernaey, John M . Woodley, Rafiqul Gani, 2011, "Design of Tailor-made Fuel Blends of Gasoline and Bio-fuels", International Congress on Sustainability Science and Engineering (ICOSSE'11), Tucson, Arizona, 9-12 January
2011-2	I. Mitrofanov, G. Sin, R. Gani, 2011, "Computer-Aided Solvent Selection Framework", CAPE forum-2011, Bradford, UK, 21-22 March
2011-3	Jakob Kjøbsted Huusom, 2011, "The Role of Mechanistic and Statistic Models in Predictive Control Applications", CAPE forum-2011, Bradford, UK, 21-22 March
2011-4	Rafiqul Gani, 2011, "Model based process-product design and analysis", ICAMAO, Kuala Lumpur, Malaysia, 19-21 April **(Plenary Lecture)**

2011-5	Nor Alafiza Yunus, Rafiqul Gani, John Woodley, 2011, "Design of Tailor-Made Chemical Blend Using a Decomposition-Based Computer-Aided Approach", ICAMAO, Kuala Lumpur, Malaysia, 19-21 April
2011-6	Azizul Mustaffa, Georgios Kontogeorgis, Rafiqul Gani, 2011, "Building a Multilevel Modeling Network for Lipid Processing Systems", ICAMAO, Kuala Lumpur, Malaysia, 19-21 April
2011-7	Noor Asma Fazli Samad, Gürkan Sin, Krist V. Gernaey, Rafiqul Gani, 2011, "Systematic Procedure for Generating Operational Policies to Achieve Target Crystal Size Distribution (CSD) in Batch Cooling Crystallization", ICAMAO, Kuala Lumpur, Malaysia, 19-21 April (**Best paper award**)
2011-8	Rafiqul Gani, 2011,"Chemical Engineering Education in a Bologna Three Cycle Degree System", AMIDIQ, Quintara Rio, Mexico, 3-6 May **(Invited Lecture)**
2011-9	Rafiqul Gani, 2011, "Systematic methods for synthesis and design of sustainable chemical and biochemical processes", AMIDIQ, Quintara Rio, Mexico, 3-6 May **(Plenary Lecture)**
2011-10	Alberto Vergara-Fernández, José Rebolledo-Castro, Ricardo Morales-Rodriguez, 2011, "Multiscale Modelling Approach for a Fungal Biofilter Unit for the Hydrophobic Abatement of Volatile Organic Compounds", XXXII National Meeting and 1st International Congress AMIDIQ-2011, Riviera Maya, Mexico, 3-6 May
2011-11	Ricardo Morales-Rodriguez, Chien-Tai Tsai, Anne S. Meyer, Krist V. Gernaey, Gürkan Sin, 2011, "Validation of Inhibition Effect in the Cellulose Hydrolysis: a Dynamic Modelling Approach", XXXII National Meeting and 1st International Congress AMIDIQ-2011, Riviera Maya, Mexico, 3-6 May
2011-12	Ricardo Morales-Rodriguez, Anne S. Meyer, Krist V. Gernaey, Gürkan Sin, 2011, "Technology Evaluation of Process Configurations for Second Generation Bioethanol Production using Dynamic Model-based Simulations", XXXII National Meeting and 1st International Congress AMIDIQ-2011, Riviera Maya, Mexico, 3-6 May
2011-13	Ricardo Morales-Rodriguez, Anne S. Meyer, Krist V. Gernaey, Gürkan Sin, 2011, "Modelling Framework for the Identification of Critical Variables and Parameters under Uncertainty in the Bioethanol Production from Lignocellulose", XXXII National Meeting and 1st International Congress AMIDIQ-2011, Riviera Maya, Mexico, 3-6 May
2011-14	Jakob Kjøbsted Huusom, 2011, "The Role of Mechanistic and Statistic Models in Predictive Control Applications", Model Based Control Conference, DTU, Lyngby, Denmark, 5 May
2011-15	Philip Lutze, Rafiqul Gani, John M. Woodley, 2011, "A systematic synthesis and design methodology to achieve process intensification in (bio)chemical processes", Process Intensification Network (PIN) – NL Spring Session, Utrecht, The Netherlands, 11 May
2011-16	Jakob Kjøbsted Huusom, Niels Kjølstad Poulsen, Sten Bay Jørgensen and John Bagterp Jørgensen, 2011, "Model Predictive Control with dead-band for uncertain time delay systems", 21th European Symposium on Computer Aided Process Engineering, ESCAPE21, Chalkidiki, Greece, 29 May -1 June

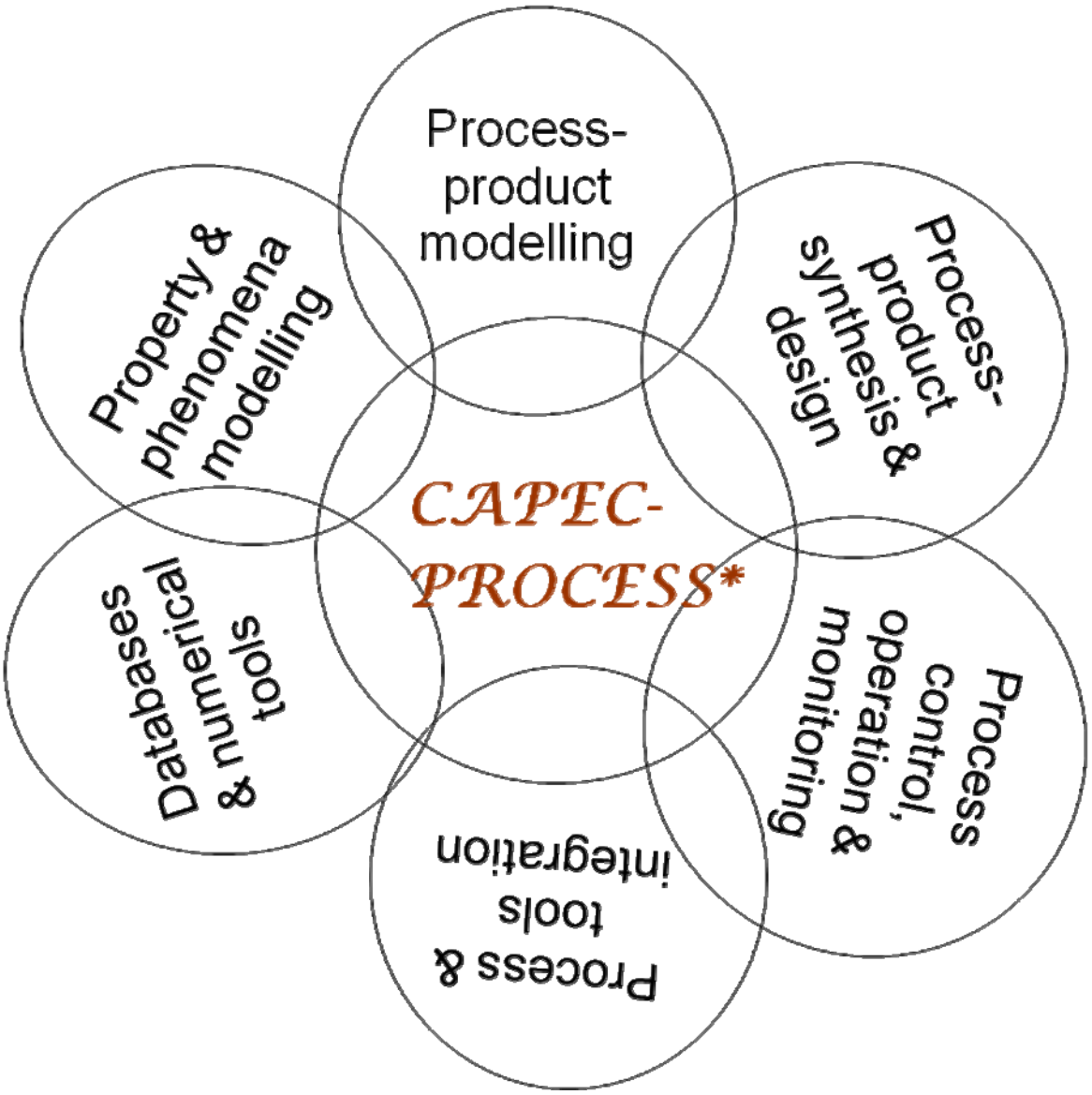
2011-17	Elisa Conte, Rafiqul Gani, 2011, "Chemicals Based Formulation Design: Virtual Experimentations", Proceedings 21st European Symposium on Computer Aided Process Engineering, ESCAPE 21, Chalkidiki, Greece, 29 May -1 June
2011-18	Chiara Piccolo, Patrick M. Piccione, Rafiqul Gani, 2011, "Modeling and design of reacting systems with phase transfer catalysis", 21th European Symposium on Computer Aided Process Engineering, ESCAPE21, Chalkidiki, Greece, 29 May -1 June
2011-19	Oscar Andres Prado-Rubio, Sten Bay Jorgensen and Gunnar Jonsson, 2011, "Systematic Procedure for Integrated Process Operation: Reverse Electro-Enhanced Dialysis (REED) during Lactic Acid Fermentation", 21th European Symposium on Computer Aided Process Engineering, ESCAPE21, Chalkidiki, Greece, 29 May -1 June
2011-20	Albert E. Cervera, Rafiqul Gani, Søren Kiil, Tommy Skovby, Krist V. Gernaey, 2010, "A systematic methodology for the design of continuous active pharmaceutical ingredient production processes", 21th European Symposium on Computer Aided Process Engineering, ESCAPE21, Chalkidiki, Greece, 29 May -1 June
2011-21	Ravendra Singh, Raquel Rozada-Sanchez, Tim Wrate, Frans Muller, Krist V. Gernaey, Rafiqul Gani, John M. Woodley, 2010, "A retrofit strategy to achieve "Fast, Flexible, Future (F3)" pharmaceutical production processes", 21th European Symposium on Computer Aided Process Engineering, ESCAPE21, Chalkidiki, Greece, 29 May -1 June
2011-22	Klaus Reinholdt Nyhuus Hansen, Martin Grunow, Rafiqul Gani, 2010, "Robust Market Launch Planning for a Muti-Echelon Pharmaceutical Supply Chain", 21th European Symposium on Computer Aided Process Engineering, ESCAPE21, Chalkidiki, Greece, 29 May -1 June
2011-23	Carlos A. Diaz-Tovar, Azizul A. Mustaffa, Amol Hukkerikar, Alberto Quaglia, Gürkan Sin, Georgios Kontogeorgis, Bent Sarup, Rafiqul Gani, 2010, "Lipid Processing Technology: Building a Multilevel Modeling Network", 21th European Symposium on Computer Aided Process Engineering, ESCAPE21, Chalkidiki, Greece, 29 May -1 June
2011-24	Brock C. Roughton, John White, Kyle V. Camarda, and Rafiqul Gani, 2010, "Simultaneous Design of Ionic Liquids and Azeotropic Separation Processes", 21th European Symposium on Computer Aided Process Engineering, ESCAPE21, Chalkidiki, Greece, 29 May -1 June
2011-25	Noor Asma Fazli Abdul Samad, Ravendra Singh, Gürkan Sin, Krist V. Gernaey, Rafiqul Gani, 2010, "Integration of Generic Multi-dimensional Model and Operational Policies for batch Cooling Crystallization", 21th European Symposium on Computer Aided Process Engineering, ESCAPE21, Chalkidiki, Greece, 29 May -1 June
2011-26	Susilpa Bommareddy, Mario R. Eden, Rafiqul Gani, 2010, "Computer Aided Flowsheet Design using Group Contribution Methods", 21th European Symposium on Computer Aided Process Engineering, ESCAPE21, Chalkidiki, Greece, 29 May -1 June
2011-27	Martina Heitzig, Christopher Gregson, Gürkan Sin, Rafiqul Gani, 2010, "Application of computer-aided multi-scale modelling framework – Aerosol case study", 21th European Symposium on Computer Aided Process Engineering, ESCAPE21, Chalkidiki, Greece, 29 May -1 June
2011-28	Mehboob Nawaz, Edwin Zondervan, John Woodley and Rafiqul Gani, 2010, "Design of a Sustainable Biorefinery", 21th European Symposium on Computer Aided Process Engineering, ESCAPE21, Chalkidiki, Greece, 29 May -1 June

2011-29	Philip Lutze, Rafiqul Gani, John M. Woodley, 2010, “Phenomena-based Process Synthesis and Design to achieve Process Intensification”, 21th European Symposium on Computer Aided Process Engineering, ESCAPE21, Chalkidiki, Greece, 29 May -1 June

	G – Invited Seminars 2010
	Rafiqul Gani, 2010, "Solvent Selection and Design", RWTH Aachen, Germany, 22 January
	R. Gani, 2010, "Solvents, green chemistry and sustainable product-process design", TU-Delft, TU-Eindhoven, University of Twente, The Netherlands, 7-9 April
	R. Gani, 2010, "A process systems engineering approach to managing the complexity in chemical product process design", Tsinghua University; Beijing, China, 14 May
	Rafiqul Gani, 2010, "Property modeling for applications in chemical product and process design", University of Ghent, Belgium, 12 July
	Rafiqul Gani, 2010, "Managing Complexity in Product Process Engineering", Mitsubishi Chemical Corporation, Kashima Plant, Kashima, Japan, 3 August
	Gürkan Sin, 2010, "Sensitivity and uncertainty analysis: Expanding engineering toolbox for science-based decision making", Kongsberg Oil and Gas Technology, Sandvika, Norway, 24 September
	Rafiqul Gani, 2010, "Design and synthesis of sustainable chemical and biochemical processes", PPC, Chulalongkorn University, Bangkok, Thailand, 5 October 2010
	Rafiqul Gani , 2010, "Managing the Complexity in Product and Process Engineering", 2010 Fall J.D. Lindsay Lecture Series, Texas A&M University, USA, 27 October
	Rafiqul Gani, 2010, "Sustainable Chemical and Bio-chemical Process Design", GlaxoSmithKline, Philadelphia, USA, 15 November
	Rafiqul Gani, 2010, "Property modelling for applications in product and process Engineering", Sogang University, South Korea, 30 November
	Rafiqul Gani, 2010, "Managing the complexity in product and process engineering", Yonsei University, South Korea, 1 December (10:00 am)
	Rafiqul Gani 2010, "Solvents, green chemistry and sustainable product-process design", Korea University, Seoul, South Korea, 1 December (5:00 pm)
	Rafiqul Gani 2010, "Sustainable design of chemical and bio-chemical processes", Korea University, Seoul, South Korea, 2 December
	G – Invited Seminars 2011
	Rafiqul Gani, 2011, "CAPEC Overview and Status - 2011", DSM, The Netherlands, 27 January
	Rafiqul Gani, 2011, "CAPEC Overview and Status - 2011", Lonza, Switzerland, 10 February
	Rafiqul Gani , 2011, "Managing the Complexity in Product and Process Engineering", Departmental Seminar, NTUA, Athens, Greece, 17 March
	Rafiqul Gani, 2011, "Building and sustaining an Industrial Consortium – The experience of DTU-CAPEC", UTM, Johar Bahru, Malaysia, 22 April 2011

Accepted/planned conference presentations between July – December 2011	
	Amol Hukkerikar, Bent Sarup, Gürkan Sin and Rafiqul Gani, 2011, ”A Systematic Methodology for Uncertainty Analysis of Group Contribution Based and Atom Connectivity Index Based Models for Estimation of Properties of Pure Components”, 25th European Symposium on Advanced Thermodynamics (ESAT), Saint Petersburg,. Russia, 24-27 June
	Jakob Kjøbsted Huusom, Niels Kjølstad Poulsen, Sten Bay Jørgensen and John Bagterp Jørgensen, 2011, ”Adaptive Disturbance Estimation for Offset-Free SISO Model Predictive Control”, American Control Conference ACC, San Francisco, USA, 29 June -1 July
	Jakob Kjøbsted Huusom, Niels Kjølstad Poulsen, Sten Bay Jørgensen, John Bagterp Jørgensen, 2011, ”Noise Modelling and MPC Tuning for Systems with Infrequent Step Disturbances”, 16th IFAC World Congress, Milan, Italy 28 August – 2 September
	Chiara Piccolo, George Hodges, Patrick M. Piccione, Rafiqul Gani, 2011, “Modelling and design of phase transfer catalytic processes”, 8th European Congress of Chemical Engineering (ECCE-8), Berlin, Germany, 25-29 September
	Chiara Piccolo, Patrick M. Piccione, Andrew Shaw, George Hodges, Rafiqul Gani, 2011, “Systematic computation of phase partition and solubilities in phase transfer catalytic processes”, 8th European Congress of Chemical Engineering (ECCE-8), Berlin, Germany, 25-29 September
	Elisa Conte, Rafiqul Gani, Peter Crafts, 2011, “A framework for API solubility modelling”, 8th European Congress of Chemical Engineering (ECCE-8), Berlin, Germany, 25-29 September
	Alberto Quaglia, Bent Sarup, Gürkan Sin and Rafiqul Gani, 2011, “A systematic framework for CAFD and resources allocation optimization using MINLP in vegetable oil processing”, 8th European Congress of Chemical Engineering (ECCE-8), Berlin, Germany, 25-29 September
	Martina Heitzig, Christopher Gregson, Gürkan Sin, Rafiqul Gani, 2011, ”Systematic multi-scale model development strategy for fragrance spraying process and transport”, 8th European Congress of Chemical Engineering (ECCE-8), Berlin, Germany, 25-29 September
	Philip Lutze, Rafiqul Gani, John M. Woodley, 2011, “Application of a Synthesis and Design Methodology to achieve Process Intensification”, 8th European Congress of Chemical Engineering (ECCE-8), Berlin, Germany, 25-29 September
	Ravendra Singh, Raquel Rozada-Sanchez, Tim Wrate, Frans Muller, Krist V. Gernaey, Rafiqul Gani, John M. Woodley, 2011, ”Substrates adoption methodology (SAM) to achieve “Fast, Flexible, Future (F^3)” pharmaceutical production processes”, 8th European Congress of Chemical Engineering (ECCE-8), Berlin, Germany, 25-29 September
	Katja Haas-Santo, Bhanu Vankayala, R. Dittmeyer, Ravendra Singh, Krist V. Gernaey, Rafiqul Gani, John M. Woodley, Raquel Rozada-Sanchez, Frans Muller, 2011, “Development of a fast and flexible generic process for the reduction of nitro compounds”, 8th European Congress of Chemical Engineering (ECCE-8), Berlin, Germany, 25-29 September

	Ricardo Morales-Rodriguez, Anne S. Meyer, Krist V. Gernaey, Gürkan Sin, 2011, "An Integral Analysis for Second Generation Bioethanol Production via a Dynamic Model-Based Simulation Approach: An Energy Efficiency Assessment", 8th European Congress of Chemical Engineering (ECCE-8)/ECAB 1, Berlin, Germany, 25-29 September
	Amol Hukkerikar, Bent Sarup, Gürkan Sin and Rafiqul Gani, 2011, "A Systematic Methodology of Uncertainty Analysis of Group Contribution Based and Atom Connectivity Index Based Models for Estimation of Properties of Pure Components", 8th European Congress of Chemical Engineering (ECCE-8), Berlin, Germany, 25-29 September



*** Systematic methods and tool**

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