Innovative & Sustainable Chemical and Process Analysis, Design & Synthesis

August, 28th – September, 1st 2017

Date: Aug 28th – Sept 1st ‘17
Place: NIT, Tiruchirappalli
India

Workshop Organizers

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Workshop Scope-Significance

Finding novel and more sustainable production systems is an important step towards addressing the grand challenges of energy, water, environment and food currently faced by modern society. Significantly better and/or new processing routes are needed to, just to name a few, convert available resources to useful products, recycle unused material, and reprocess used material, without negatively impacting sustainability of modern society. The synthesis-design of processing routes is receiving increasing attention, not only due to the scope and significance of the problems that it covers, but also because of its industrial relevance. A processing route is a combination of raw materials, a series of processing steps to convert them, and products which they can be converted to; each processing step has various alternatives in terms of processing technologies, giving rise to a superstructure of alternatives. The synthesis-design problem is formulated as a superstructure optimization problem, solved in 3-stages. Stage-1 is the synthesis stage where a preliminary processing route is identified together with interesting alternatives. Stage-2 is the design-analysis stage where a detailed design is performed on the processing route from stage-1. Analysis of the design is performed to identify process “hot-spots” that help to define targets for improvement. Stage-3 is the innovation stage, where new alternative processing routes that match the targets of improvement are identified, thereby leading to innovative and sustainable process design. A computer-aided flowsheet design tool (ProCAFD), which performs the 3-stages innovative sustainable process synthesis, design and analysis in 12 hierarchical tasks will be used.

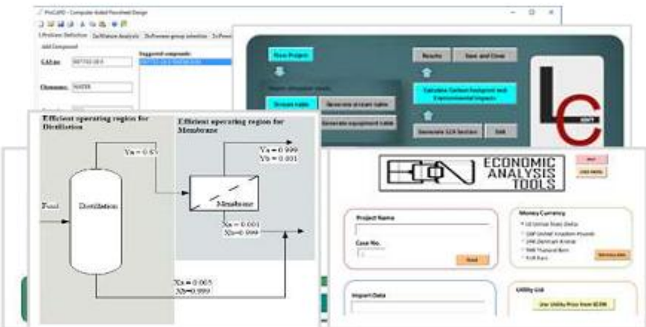
Program Schedule:

	Lecture	Topic	Remarks
Day 1 09:00-12:00	0	Introduction to innovative and sustainable process design, synthesis and analysis	Introduction to concepts, methods, tools
	1	Task-1 (problem definition) & Task-2 (problem analysis)	ProCAFD (steps 1-2)
14:00-17:00	2	Task-3 (processing route synthesis) – group contribution method	ProCAFD (steps 3-5)
Day 2 09:00-12:00	3	Task-3 (processing route synthesis) – superstructure optimization	Super-O
14:00-17:00	4	Task-4 (process design & simulation) – simple model	ProCAFD (step 6)
	5	Tasks 5-6 (process design & simulation) - process design	ProCAFD (step 6)
Day 3 09:00-12:00	6	Task-7 (process design & simulation) - rigorous simulation	ProCAFD (step 7)
14:00-17:00	7	Task-8 (process analysis) sizing & costing	ECON
Day 4 09:00-12:00	8	Task-9 (process analysis) economic evaluation	ECON
14:00 – 17:00	9	Task-9 (process integration)	ProCAFD-tools
Day 5 09:00-12:00	10	Task-11 (process final design analysis) sustainability and lifecycle analysis; identify process “hot-spots”	PROII/ASPEN/Sustain Pro/LCSoft
14:00-17:00	11	Task-12 (process optimization)	PROII/ASPEN
	12	Summary – conclusions	

** All sessions (morning & afternoon) have tutorial exercises. Lunch Break: 12.00 – 14.00*

Computer-Aided Tools

- ProCAFD – Computer aided flowsheet design
- ECON – Economic Analysis Tool
- SustainPro- Sustainability Analysis Tool
- LCSoft- Life Cycle Analysis Tool
- Super-O – Superstructure Optimization



Task 1: Identify (through a search of publicly available information) details about your chemical product. Collect useful information about your product – for example, why is the product important? What are its uses? What are its characteristic properties? Who are the biggest producers?

Task 2: Collect as much information you can find for the process you have chosen (based on the reaction steps) to make your product. You need to decide about the additional details of the raw material (that should be used) and the product quality – check also the process design document for additional (specified) details about the product and the raw material.

Task 3: Use an appropriate method for process synthesis to generate feasible processing routes and select one for further investigation. The use of a process group contribution method and a superstructure based optimization method will be highlighted in this task. ProCAFD will help you to perform process group based flowsheet (processing route) generation. Also, a superstructure based optimization to find the optimal processing route will be employed through Super-O software.

Task 4: Perform a mass balance on the process flowsheet you have selected. Note that before you can complete a mass balance, you will need to make a number of design decisions and you will need a model for performing mass balance calculations. ProCAFD will help you to model and perform simple mass and energy balance calculations.

Task 5: Add temperatures and pressures on every stream-operation to perform a mass and energy balance with the simple model. ProCAFD will help you to perform these calculations.

Task 6: Using the results from task 5 as the basis, perform mass and energy balances using the simple process model from task 4. Also, energy (heat) added or removed from each unit operation will be calculated. ProCAFD will help to perform these calculations.

Task 7: The simple models are now replaced with more rigorous models so that the mass and energy balances can be performed with more detailed design. ProCAFD will help to determine the process designs and launch the PROII simulator for rigorous process simulation.

Task 8: Using the results from Task 7, equipment sizing and costing calculations are now performed for all equipment in the process flowsheet. A number of new design decisions need to be taken here. The sizing and costing values will indicate if the earlier decisions need to be changed, and previous steps (tasks) need to be repeated. The ECON software tool can be used for these calculations.

Task 9: Using the results from Task 8, perform an economic evaluation of the design process. Here you will need to use data you collected before on costs, as well as new data that will need to be obtained. The results will indicate if the decisions taken previously are still reasonable. If yes, then you have an acceptable "base case" design. ECON is used for this task.

Task 10: Using the results of Task 9, investigate if opportunities for heat and mass integration exist. If yes, apply them. This will reduce the operating (manufacturing) cost and therefore, the process economics will improve. PROII and tools from ProCAFD is used in this task.

Task 11: Using the updated process (design) flowsheet from Task 10 as the basis, perform environmental impact and sustainability calculations to verify if your design decisions are also acceptable from an environmental point of view. See supplied notes for environmental impact analysis. SustainPro (for sustainability analysis) and LCSoft (for life cycle assessment) are employed here.

Task 12: Investigate if the base case design (plus changes due to mass/heat integration) at the end of Task11 can be further improved. Formulate a process optimization problem to improve the profit further, without making the environmental impact worse than the design at the end of Task 11.

Who Should Attend?

- Process Engineer, Chemical Engineer, Process Technologist
- R&D Teams, Consultant, Researcher, Chemist
- Professor/Lecturer, Students working in process synthesis, design development

List of Publications

- A.K. Tula. *Computer-aided Sustainable Process Synthesis-Design and Analysis*. PhD-thesis, Technical University of Denmark, Lyngby, Denmark. (2016)
- A.K.Tula, B.Bridgette, N. Garg, K.Camarda, R. Gani. *Sustainable Process design & analysis of hybrid separations*. Computers & Chemical Engineering, 39 (2017): 61-94
- A.K. Tula, M. R. Eden, and R. Gani, 2015, *Process synthesis, design and analysis using a process group contribution method*, Computers. Chem. Eng., 81, 245-259.
- D.K. Babi, J. Holtbruegge, P. Lutze, A. Gorak, J.M. Woodley, R. Gani,. 2015. *Sustainable Process Synthesis-Intensification*. Comput. Chem. Eng., 81: 218–44.
- A.Carvalho, H.M. Matos, R.Gani, 2013 *SustainPro - A tool for systematic process analysis, generation and evaluation of sustainable design alternatives*, Comput. Chem. Eng., 50, 8-27

Workshop Lecturers

Prof. Rafiqul Gani is professor of system design at the Department of Chemical and Biochemical Engineering, The Technical University of Denmark and the former head and co-founder of the Computer Aided Process Engineering Center (CAPEC). His current research interests include development of computer aided methods and tools for modelling, property estimation, process-product synthesis & design, and process-tools integration. He has published 406 peer-reviewed journal-proceedings articles and book chapters, and, delivered over 350 lectures, seminars and plenary/keynote lectures at international conferences, institutions and companies all over the world. Professor Gani is the president of the EFCE (European Federation of Chemical Engineering), elected for a second term 2016-2018; a Fellow of the AIChE and also a Fellow of IChemE. He is a co-founder and the CEO of the PSE for SPEED (Sustainable Product Process Engineering, Evaluation and Design) company.

Anjan Tula is a Postdoctoral Researcher at the Department of Chemical Engineering, Auburn University and the Head of Process Engineering Division of the PSE for SPEED (Sustainable Product Process Engineering, Evaluation and Design) company. His main area of expertise is in development of computer-aided methods for process synthesis and innovation. Anjan has a doctorate degree in chemical engineering from Technical University of Denmark and prior to that he has 3-year's work experience in General Electric as process engineer. As a part of his PhD he has developed computer-aided method and tool for systematic process synthesis-design & analysis of chemical and biochemical processes. His works has been awarded and widely accepted and published in several international conferences and journals.

Registration:

The Registration fee is as follows:

Industry/ Research Organizations:	**Rs. 20,000/-**
Faculty:	**Rs. 6,000/-**
M.Tech Students & Research Scholars:	**Rs. 3,000/-**

The Registration fee includes all instructional materials, computer use for tutorials and Boarding and lodging which will be provided in Institute Guest House/Hostels. Interested persons can apply along with the requisite Demand Draft drawn in favor of "Director, NIT Tiruchirappalli", payable at Tiruchirappalli. If you are a student/scholar, your application must be endorsed by the Head of the Department. For detailed information, you may visit: http://iscpads2017.nitt.edu

ABOUT THE INSTITUTE

National Institute of Technology, Tiruchirappalli (NITT) , is one among the premier Institutions of India and is well known for its high standards in teaching and research. It has been declared as an Institute of National Importance by the Government of India under NIT Act. According to the Ministry of Human Resources Development, NIRF 2017, NIT Trichy has been ranked as the 1st NIT among all the NITs and 11th among all the technical institutes in India. The Institute has signed MoUs with various Industries and Institutions both in India as well as in abroad to promote collaborative research and consultancy. It has been awarded the "Best Industry linked National Institute of Technology in India" by the Confederation of Indian Industry (CII) in the year 2015.

Chemical Engineering Department

Established in 1968, the Department of Chemical Engineering, NIT Trichy is regarded as one of the premier centers for Chemical Engineering in India by industries as well as academia. It also has the distinction of being ranked as one of the top seven Chemical Engineering divisions in India. The department has expertise in Process Modeling, Control and Simulation, Advanced Separation Technology, Bio Fuel Cells and Particulate Technology supporting the needs of process industry and development of skilled human resources both at UG and PG/ Research level. The department has facilities for experimental investigation and also has access to commercial software for simulation of process dynamics and analysis.

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