COURSE TITLE: Computer Aided Simulation of Chemical Processes

NIT Warangal

22-27 November 2016

1.0 Overview

Process simulation is a discipline transversal to all the areas of chemical engineering. The development of many engineering projects demand simulation studies since the preliminary feasibility analysis, conceptual design, detailed design, until the process operation. The generation of new process requires the integration of concepts of chemical engineering. All that integration redounds in controllability studies and dynamic analysis, energy integration and optimization, which aim to achieve the goals of environmental protection, process safety, and product quality.

Chemical process simulation aims to represent a process of chemical or physical transformation through a mathematical model that involves the calculation of mass and energy balances coupled with phase equilibrium and with transport and chemical kinetics equations. All this is made to predict the behavior of a process of known structure, in which some preliminary data of the equipment that constitute the process are known. The mathematical models employed in process simulation contain linear, nonlinear, and differential algebraic equations, which represent equipment or process operations, physical–chemical properties, connections between the equipment and operations and their specifications.

Process simulation is a core activity in R & D, Design and Operation. Process simulation can be used to effectively design a new process, i.e., to determine the size of equipment in a chemical plant, the amount of energy needed, the overall yield, the magnitude of waste streams generated and the profitability analysis. It can also be used to evaluate alternate plant configurations, modernizing and revamping existing plants, debottlenecking, assist in planning for production changes and assessing the compliance with environmental regulations.

As the results of process simulation depend upon thermodynamics and transport processes, the mathematical models are complicated and would be time-consuming to solve without the use of a computer. **This course emphasizes the use of a process simulator, such as Aspen Plus & PROII, to carry out process simulation and is designed to give rich hands on experience to participants in the use of a process simulator. The exercises chosen during the laboratory sessions range from simple problems encountered in day to day life to practical/industrial problems.**

2.0 Objectives

The primary objectives of the course are as follows:

i) Expose the participants to the fundamentals of Process simulation, its pre-requisites and challenges.
ii) Provide hands on experience to the participants in the application of a Process Simulator for simulating any chemical process.
iii) Provide exposure to practical/industrial problems and their solutions, through case studies and live projects.
iv) Train the participants in the advanced applications of process simulators such as detailed design of process equipment, dynamic simulation, heat integration and Heat Exchanger Network design, Economic analysis and developing custom models.

3.0 Course tutors

Professor Rafiqul Gani (Technical University of Denmark, Denmark)
Dr. Deenesh T Babi (Novo Nordisk, Denmark)
Dr. A. Sarath Babu (NIT Warangal, India)
Dr. V. Ramsagar (NIT Warangal, India)

4.0 Course details

4.1 Course Duration: 1 week (6 working days) 22-27 November 2016

4.2 Lecture-tutorial schedule:

Date	Day	Time	L/T/P	Topic
22 Nov (Introduction of concepts, methods and tools)	1	09:00 to 10.45	L1	Introduction to simulation of chemical processes (*R Gani*)
		11:00 to 12:45	L1a	Introduction to process simulation and ist prerequisites (*NIT host faculty*)
		14:00 to 17:00	T1	Tutorial session-1: Introduction to process simulators; problem definition; thermodynamic model selection; unit operation model selection (*D Babi plus NIT host faculty & R Gani*)
23 Nov (Modelling & related issues; Single issues)	2	09:00 to 10.45	L2	Modelling and related issues: model structure, model analysis, different types of models (*R Gani*)
		11:00 to 12:45	L2a	Degrees of freedom analysis; custom modeling (*NIT host faculty*)
		14:00 to 17:00	T2	Tutorial session-2: Use of simple models; use of rigorous models; thermodynamic properties evaluation; simulator specifications (*D Babi plus NIT host faculty*)
24 Nov (Problem solving strategies; Process flowsheet issues; incremental problem solution)	3	09:00 to 10.45	L3	Simulation problem decomposition and simulation strategies (*R Gani*)
		11:00 to 12:45	L3a	Approaches to simulation: sequential modular approach, equation oriented approach – challenges (*NIT host faculty*)
		14:00 to 17:00	T3	Tutorial session-3: process simulation broken down into tasks – simple mass balance; setting of temperature & pressure; mass + energy balance with simple model; rigorous simulation (*D Babi plus NIT faculty & R Gani*)
25 Nov (Numerical methods - simulation & optimization)	4	09:00 to 10.45	L4	Simulation strategies – numerical issues (*R Gani*)
		11:00 to 12:45	L4a	Mathematical methods specific to simulation, dynamic simulation (*NIT host faculty*)
		14:00 to 17:00	T4	Tutorial session-4: Choice of numerical solvers; setting-up optimization problems; dynamic simulation (*D Babi + NIT host faculty & R Gani*)
26 Nov (Process & tools integration)	5	09:00 to 10.45	L5	Integration: concepts, methods & tools (*R Gani*) & sustainable process design (*D Babi*)
		11:00 to 12:45	L5a	Heat exchanger networks, solids handling, dynamic simulation (*NIT host faculty*)
		14:00 to 17:00	T5	Tutorial session-5: Integration of analysis tools - ECON, SUSTAIN-Pro & LCSoft & simulator based tutorials for heat exchanger networks, Cost estimation (*D Babi + NIT host faculty & R Gani*)
27 Nov (Introduction	6	09:00 to 10.45	L6	Computer aided flowsheet design and computer aided chemical product design with illustrating case

to new class of simulation based tools and case studies)				studies (*R Gani*)
		11:00 to 12:45	L6a	Case Studies of Practical/Industrial problems (*NIT host faculty*)
		14:00 to 15:00	T6	Examination for Students (*NIT host faculty*)
Course review		16:00 – 17.00		Discussion between participants and course tutors

4.3 Useful references (books & published papers)

- Lorenze T. Biegler, Ignacio E. Grossmann and Arthur W. Westerberg: Systematic *Methods of Chemical Process Design*, Prentice Hall, 1997.
- **Warren D. Seider, J. D. Seader, Daniel R. Lewin, S. Widegado, Rafiqul Gani, Ka M. Ng *Process Design Principles: Synthesis, Analysis and Evaluation*, John Wiley & Sons Ltd, 2015 (4th Edition).**
- Max S. Peters and Klaus D. Timmerhaus, *Plant Design and Economics for Chemical Engineers*, 4th Edition, McGraw-Hill, 2010.
- Robin Smith, *Chemical Process Design and Integration*, John Wiley & Sons, Ltd, 2005.
- Supplied lecture notes, published papers