Indian Institute of Technology Kanpur

Proposal for a New Course

1. **Course No:** CHE 6XX
2. **Course Title:** Advanced topics in process modelling and simulation
3. **Course Credits (9):** 2-0-3-0 (2L, 0T, 3P, 0A)
4. **Pre-requisites:** None
5. **Course Duration:** Full Semester
6. **Level of the course:** Graduate/Department Elective
7. **Proposing department:** Chemical Engineering
8. **Proposing Instructor(s):** Raghavendra Ragipani
9. **Other faculty members interested in teaching the proposed course:** Ishan Bajaj, Dipin Pillai, Harshwardhan Katkar
10. **Course Description:**
    A. **Objectives:** This is an advanced hands-on course on process modelling & simulation using Aspen Plus. Students will learn about property estimation, multicomponent & multiphase flash calculations, phase stability algorithms, equilibrium and rate-based modelling for steady-state and dynamic processes. Students will be familiarized with tools such as sensitivity analysis, parameter estimation, and process optimization. At the end of this course, students will be able to perform process simulations for design, rating, and optimisation.
    B. **Contents:** Lecture-wise break-up (considering the duration of each lecture is 50 minutes)

S No	Broad title	Topics	No. of lectures
1	Introduction to process modelling and simulation	• Why study process simulations? Introduction to systems approach • Sequential Modular (SM) and Equation Oriented (EO) flow sheeting • Making of a good process simulator – modelling strategies, convergence strategies for SM simulations with recycles, and computation efficiency	2
2	Thermodynamics for process simulations	• Overview of property models for various fluids • Verifying pure component properties • Verifying multicomponent electrolyte and non-electrolyte mixture properties – mixing laws for EOS, excess GFE models, local composition models • Binary interaction parameter estimation by regression	3
3	Computational strategies and advanced unit operation modelling	• Algorithms for flash calculations and phase stability criteria • Process flowsheet convergence • Data reconciliation • Data regression	6

		• Measurement model • Handling optimisation problems • Troubleshooting convergence problems • Custom model development	
4	Equilibrium & stage-based modelling	• Algorithms for non-isothermal stage-based modelling • Chemical equilibrium calculations – non-electrolyte and electrolyte systems • Complex configurations	4
5	Rate-based simulations	• Rate-based models for heterogeneous catalytic reactors • Absorption with reaction – mass transfer models and enhancement factor • Fit kinetic parameters	5
6	Dynamic processes	• Modelling cyclic adsorption – breakthrough studies, cyclic steady state	3
7	Handling solids	• Solids processing – stream classes, particle size distributions	2
8	Surrogate models	• Use of surrogate models – sampling methods, and training neural networks	3
	Total Lectures		**28**

C. Suggested simulation exercises:

1. Pure component property estimation (T-S plot) for designing a Rankine-cycle power plant/Organic Rankine cycle waste heat recovery unit.
2. Simulating a multi-stage flash distillation unit for desalination of water.
3. Determination of binary interaction parameters by regression – ethanol-water VLE, non-condensable gas solubility in solvent, salt solubility in aqueous solution etc.
4. Multicomponent property estimation for designing reactor-separation loops.
5. Phase stability – heptane-methanol mixture.
6. Steady-state simulation of azeotropic distillation of ethanol-water mixture.
7. Rigorous design and rating of a distillation column for an increase in throughput.
8. Rate-based model for designing non-isothermal heterogeneous catalytic reactor using LHHW kinetics.
9. Evaluating performance of a reactive absorption column for acid gas scrubbing.
10. Custom model for a membrane separation unit.
11. Unsteady-state simulation of pressure-swing adsorption process for gas purification.
12. Modelling a solid drying process.
13. Simulation of a particulate process with polydisperse particles.
14. Process optimization with surrogate models.
15. Data reconciliation using actual plant data.
16. Model batch production of a fine chemical.

D. Short summary for including in the course booklet:

Process modelling and simulation tools are widely used in chemical industries for process design, troubleshooting, and optimization. This course provides hands-on experience of process modelling and simulation for chemical engineering graduate students. Modelling and simulation of industry

relevant processes such as distillation, reactive absorption, pressure-swing adsorption, multiphase reactors will be considered. Students will learn about performance rating, sensitivity analysis, process optimsation, and parameter estimation.

11. Recommended books:
- Selected research articles
- User manuals for Aspen Plus and Aspen Adsorption.
- Selected chapters from Chemical Thermodynamics for Process Simulation, 2nd Edition, Wiley, by *Jürgen Gmehling, Michael Kleiber, Bärbel Kolbe, Jürgen Rarey*, Chemical Reactor Analysis and Design, 3rd Edition, Wiley, by *Froment, Bischoff, De Wilde*, and Principles of Adsorption and Adsorption Processes, Wiley, by *Doughlas M. Ruthven*.

12. Other remarks: None

Dated: 11/08/2025

Proposer: Raghavendra Ragipani

Dated:

DPGC Convenor:

The course is approved/ not approved

Chairman, SUGC/SPGC

Dated: