

CHEN 4460 - PROCESS SIMULATION, SYNTHESIS, AND OPTIMIZATION (2)
Required Core Course

2009-2010 Catalog Data	Lec (1), Lab (3). Fundamentals of computer-aided simulation and synthesis. Process integration and optimization principles including their applications in design, retrofitting and operation of chemical processes.
Prerequisites	Pr: CHEM 2080 and completion of CHEN 3370, CHEN 3650, CHEN 3660, and CHEN 3700 with grades of C or higher.
Schedule	One one-hour lecture session and two 75-minute lab sessions per week
Course Objectives	This course is intended to introduce students to the fundamentals of computer-aided process synthesis, simulation, analysis and optimization. In particular, the course presents systematic tools for developing and screening potential process flowsheets. Students use a commercial process simulator (ASPEN PLUS) to aid in evaluating a variety of these process designs. Practical problems are used as examples. These problems include mass integration, heat-integration, separation processes and environmentally benign designs. Using a commercial solver package (LINGO) students are introduced to the formulation and solution of linear and nonlinear mathematical optimization problems for chemical engineering applications.

Textbooks

Seider, Seader, Lewin and Widagdo, Product and Process Design Principles: Synthesis, Analysis, and Evaluation, 3e, 2008, 9780470048955, Wiley
Eden, ASPEN Lab Notes, Auburn University

Lecture Topics:

1. Introduction to CHEN 4460: Course objectives, introduction of multimedia package, design and synthesis process (1 week)
2. Process creation: Preliminary database creation (1 week)
3. Heuristics for process synthesis: Reaction, mixing and recycle, separation, temperature – pressure - phase change, task integration (3 weeks)
4. Algorithmic methods for process synthesis: Reactor design, reactor network synthesis, synthesis of separation trains, sequencing of ordinary distillation columns (3 weeks)
5. Separation of non-ideal mixtures: Azeotropy, residue curve maps, distillation boundaries (2 weeks)
6. Heat and power integration: Thermal pinch analysis, heat exchanger network synthesis (3 weeks)
7. Mathematical optimization: Formulation and solution of LP, NLP, MILP, MINLP problems (2 weeks)

Lab Topics:

1. Principles of flowsheet simulation: Getting started in Aspen, problem set up, convergence (2 weeks)
2. Heat transfer: Pumps, compressors, expanders, shell-and-tube heat exchangers (2 weeks)
3. Thermodynamic analysis: Choosing property estimation methods, generating equilibrium diagrams, property data regression (2 weeks)
4. Separations: Flash operations, shortcut and rigorous fractionation/distillation models (2 weeks)
5. Reactions: Stoichiometric reactors, equilibrium reactors, PFR, CSTR (2 weeks)
6. Optimization: Introduction to LINGO, solution of LP, NLP, MILP, MINLP problems (2 weeks)
7. Simulation project: Flowsheet simulation with multiple unit operations, sensitivity analysis, heat integration and optimization (3 weeks)

Course Outcomes: Upon successful completion of this course, students should be able to:

1. Describe the more widely used industrial separation methods and their basis for separation.
2. Apply heuristics and systematic methods to narrow the search for a near-optimal sequence of distillation-type separations.
3. Sketch residue curve maps on a ternary phase diagram and define the range of possible distillation product compositions for a given feed composition.
4. Define the process flow diagram for a heterogeneous azeotropic distillation system.
5. Define the process flow diagram for a pressure swing distillation system.
6. Design and sequence distillation columns for azeotropic distillation of binary mixtures through analysis of residue curves and distillation boundaries.
7. Perform graphical and algebraic thermal pinch analysis to identify optimal heat recovery strategies for minimization of external heating and cooling requirements.
8. Synthesize heat exchanger networks that match specified process constraints and objectives with minimum total annualized cost and choose the best solution from the generated alternatives.
9. Apply state of the art mathematical programming techniques for solving LP, NLP, MILP and MINLP problems.
10. Set up a simulation model with the appropriate chemical components, unit specifications and choice of thermodynamic model and subsequently perform rigorous steady state simulation, using a commercially available process simulator, of individual process units such as compressors, flash columns, reactors, absorbers, strippers and distillation columns for binary as well as multi-component mixtures.
11. Optimize the individual units by identifying design variables available for manipulation and thereby evaluate and suggest design changes based on base case simulation results.
12. Simulate entire process flowsheets with multiple units and validate design suggestions obtained by performing energy pinch analysis.
13. Perform plant-wide sensitivity analysis to investigate the impact of certain process parameters on the overall performance.

Contribution of Course to Meeting ABET Criteria 5 (Curriculum)		
Math and Basic Sciences	Engineering Topics	General Education
0 Credits	2 Credits	0 Credits

Relationship of Course to Program Outcomes (PO's)												
Program Outcome	A	B	C	D	E	F	G1	G2	H	I	J	K
Level of Coverage	S	R	S	R	R		I	I		I		S

Date of Preparation and Person(s) Preparing This Description

February 6, 2010: Mario R. Eden