CHEM ENG 740W – Fall 2019 Syllabus

Advanced PSE Tools and Methods

McMaster University ENGINEERING

Description

Advanced techniques for modeling, design, and analysis of chemical processes. Technoeconomic analyses. Synthesis and optimization of superstructures. Life cycle assessments. Combining computer-aided process engineering software for advanced problem solving approaches, such as GAMS, gProms, and Aspen Dynamics.

Learning Objectives

The purpose of the course is to provide students with a background in some of the advanced process systems engineering techniques used in the industry. This includes common software for simulations, modeling, optimization, economic analyses, and life cycle analyses. Some prior knowledge about common tools learned in most undergraduate curricula is assumed (Aspen Plus or similar, Matlab, GAMS). Students who complete this course successfully should:

- Be familiar with the most common tools and methodologies for conducting techno-economic analyses and life cycle analyses which are of penultimate importance to today's process systems engineer.
- Understand a variety of approaches and frameworks for a variety of modeling and simulation problems and decide upon the best choice for a given type of problem.
- Be able to identify which existing software tools might be best suited to solve a chemical engineering problem.
- Throughout the course, students will be pushed to challenge ideas and norms and improve their independent critical thinking skills. This course is suitable for graduate students in any year of their program.

Course Details

Instructor: Dr. Thomas A. Adams II
tadams@mcmaster.ca

Units: 1.5 (quarter course!)

Website: On Avenue to Learn
avenue.mcmaster.ca

Lectures: TBD
Sept – Early Nov

Office Hours: JHE-371, TBD
appointments also welcome

Materials: Tutorials, assignments, readings, announcements, and solutions will be posted on the course website. Grades will be posted but are not official.

Laptops: Feel free to bring your laptops to each class, but not required.

Textbook: None

Demonstration of Knowledge

In order to demonstrate these objectives, a student should be able to:

- Perform simulations using any of the commercial software tools discussed
- Build models using both mathematical and black box frameworks
- Apply optimization algorithms toward problems built upon models of various types.
- Perform a life cycle analysis
- Perform a techno-economic analysis

Course Policies

Grading Policies

- Late submissions are docked 25% of points earned per day of lateness. Nothing is accepted after solutions have been posted.
- Valid MSAF forms for missed assignments will usually result in a deadline extension or weight-transferring into the other assignments.
- Final percentage grades will be converted to letter grades according to normal University policy.
- The instructor reserves the right to "curve" grades in your favour and to correct any grading errors, favourable or not.
- All assignments and projects are done on an individual basis.

Course Materials

There is no textbook assigned to this course, although suggested reading material will be provided. Relevant literature will include selected journal articles, textbook chapters, user manuals, etc. Any software not available to the students for free (or as a part of their normal research programs) will either be made available in the UTS or via an alternative arrangement.

Academic Honesty

- All homework is to be done individually, with no collaboration with anyone.
- Plagiarism, improper collaboration, copying unauthorized tests or aids, and other academic dishonesty will not be tolerated. **Your first offence will be reported** to the Office of Academic Integrity.
- The default penalty for academic dishonesty is a zero on the entire exam / quiz / project, even if the dishonesty occurred on just one portion or question of that exam / quiz / project. However, if Academic Integrity chooses to hold a hearing, they determine the penalty which replaces the default penalty.

Note: You are expected to exhibit honesty and use ethical behaviour in all aspects of the learning process. Academic credentials you earn are rooted in principles of honesty and academic integrity. Academic dishonesty is to knowingly act or fail to act in a way that results or could result in unearned academic credit or advantage. This behaviour can result in serious consequences, e.g. the grade of zero on an assignment, loss of credit with a notation on the transcript (notation reads: "Grade of F assigned for academic dishonesty"), and/or suspension or expulsion from the university.

Recommended Reading

Seider, Seader, Levin and Widago, Process and Product Design Principles, 3rd Ed, *Wiley 2009*. Especially chapters 22, 22S and 23 (profitability and cash flow analyses, Icarus guidebook). See also CD rom for tutorials in using Aspen Plus and Aspen Dynamics. Available in library on reserve.

Turton, Baillie, Whiting, and Shaeiwitz. Analysis, Synthesis, and Design of Chemical Processes, 3rd Ed, *Prentice Hall 2009*. See especially chapter 2. Available in library on reserve.

Towler and Sinnott. Chemical Engineering Design: Principles, Practice and Economics of Plant and Process Design. 2nd Ed, *Elsevier 2012*. See especially chapter 7. Available in library on reserve

Jimenez-Gonzales and Constable. Green Chemistry and Engineering. Wiley, 2011. See especially chapters 16 and later. Available on e-book from McMaster Library website.

Luyben WL. Distillation Design and Control Using Aspen Simulation, Wiley (2006). ISBN 9780471785248. Available on e-book from McMaster Library website.

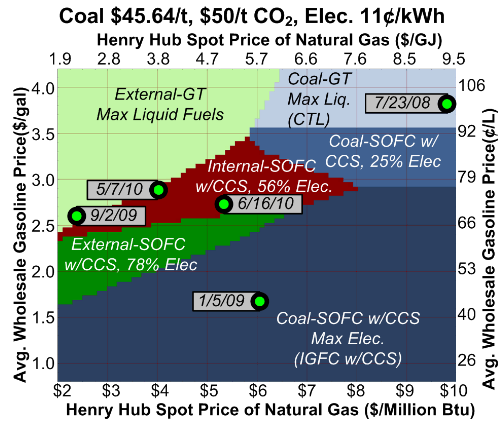
More recommendations to be posted on course website.

Grading Breakdown

Weight	Component	Comments
20%	Assignment 1	Economic and Life Cycle Analysis
20%	Assignment 2	Modelling with Aspen Dynamics
20%	Assignment 3	Modelling with gProms or Aspen Custom Modeller
20%	Assignment 4	Surrogate Modelling
20%	Assignment 5	Particle Swarm Optimization

Course Calendar *(subject to change!)*

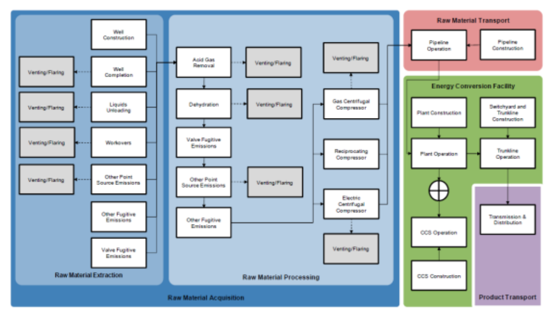
Note: Registrar has not yet scheduled rooms / days / times for this course.



1. Techno Economic Analyses

Crash course in the business economics of chemical plants. Focus is on advanced tools and methods for conducting a net present value analysis and sensitivity analysis, and extracting data from simulations.

Day	Topic	Time	Room
	1.1: Capital cost crash course. Using cost indices, labour modifiers, etc. Power law rules, approximations, and heuristics. Extrapolations from published data.		
	1.2: Standard economic analysis approaches. Profitability comparisons, net present value analyses. Financing, debt, equity, return rates. Capacity factors, inflation. Sensitivity analyses.		
	1.3: LAB: Using Aspen Icarus for capital cost predictions		
Homework 1 Part 1 provided			



2. Life Cycle Analyses

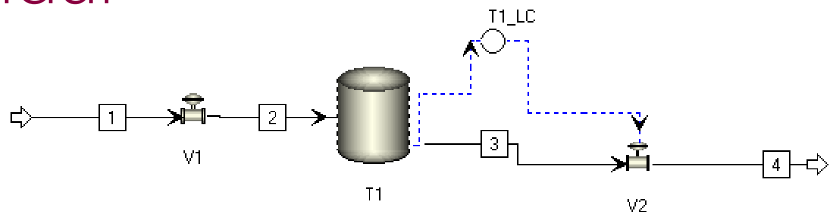
Crash course in conducting life cycle analyses using ISO 14044 and ReCiPe standard methods.

Day	Topic	Time	Room
	2.1: Life cycle boundaries. Creating supply chains. Elementary flows, resource flows, and waste flows. ISO 14044 standards for boundary definitions. Lifecycle inventories		
	2.2: Life cycle impact assessments. Midpoint vs. endpoint methods. ReCiPe. Traci. Eco 99. Tradeoff between science and emotion.		
	2.3: LAB Using OpenLCA to compute life cycle inventories and perform life cycle impact analyses.		
Homework 1 Part 2 provided. Due date TBD.			

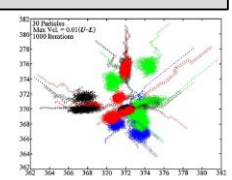
Course Calendar *(subject to change!)*

3. Dynamic Modelling

Advanced CAPE tools for dynamic modelling. gProms, Jacobian, Aspen Dynamics, Aspen Custom Modeller.



Day	Topic	Time	Room
	3.1: gProms and Jacobian. Basic ODE integration for custom models. Built-in models and tools. High index issues. PDE models. Grid discretization methods.		
	3.2: Aspen Dynamics. Integration with Aspen Properties and Aspen Plus. Flow-driven and pressure-driven simulations. Initialization via sequential-modular flowsheeting. External automation with Excel and VBA.		
	3.3: LAB: Using Aspen Dynamics		
Homework 2 Assigned			
	3.4: Aspen Custom Modeller. ODE integration. Ports, icons, model library customization. Aspen Properties and built-in streams and types. Automatic differentiation for PDE problems.		
	3.4: LAB: Using Aspen Custom Modeller		
Homework 3 Assigned			
	3.5: BR&E ProMax. Gas sweetening. CO_2 capture.		



4. Black Box Models

Black box models, reduced order models, and black box optimization

Day	Topic	Time	Room
	4.1: Regression-based models. Linear-in-the-parameters and non linear approaches. Trainings vs. testing sets. Selecting model structures. Practical applications.		
	4.2: LAB: Creating reduced models from simulations.		
Homework 4 Assigned			
	4.3: Artificial Neural Networks. Theory and CAPE tools for model construction. Data sampling and design of experiments. Latin Hypercubes.		
	4.4 Particle swarm optimization. Theory and practical applications.		
	4.5: LAB: Hands-on PSO applications.		
Homework 5 Assigned			
	4.6 TBD		