

CHE 3G04 – Winter 2017 Syllabus

Simulation, Modeling, and Problem Solving

Description

Chemical process simulations including models for separators, reactors, heat exchangers, heat integration, pressure handling, energy conversion, and other unit operations. Using process simulations to solve problems related to chemical processing, energy, and sustainability.



Learning Objectives (brief)

Students who complete this course should be able to use chemical process flowsheet simulations to solve problems in the chemical industry. This includes:

- Starting with a chemical or business objective (e.g., create so much of product A from raw materials B), **synthesize a flowsheet on paper which could achieve this objective**
- Implement** this flowsheet in a simulation program such as Aspen Plus.
- Make use of thermophysical property models in the flowsheet. This includes **identifying** the correct **models** to use.
- Make use of **unit operation models** which are built in to the software for common units such as heat exchangers, distillation columns, pumps, compressors, reactors, and mixers.
- Construct custom models** for unit operations which are not built into the software, and integrate them into the flowsheet.
- Successfully run** the flowsheet **simulation** to compute the mass and energy balances throughout.
- Extract useful information from the results** and apply it towards the solving of the original problem.
- Perform advanced functions** such as sensitivity analyses, case studies, or optimization to re-use the flowsheet thousands of times over and get an incredible amount of useful data.
- Use the results of these flowsheet simulations to **compute capital costs, energy costs, operation costs, and emissions to the environment**.
- Use these cost and impact results to make an **assessment** of the sustainability of the process using the **triple-bottom-line of sustainability** approach.

Course Details

Instructor: Dr. Thomas A. Adams II
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Website: On Avenue to Learn

Teaching Assistants:

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Lectures: Mo, We Th 5:30-6:20 T13/127

Tutorials: T1: Mo 2:30-4:20 BSB/249
T2: Tu 9:30-11:20 BSB/244
T3: We 9:30-11:20 BSB/244

Office Hours: JHE-371, Fridays, 10-11a

Prerequisites: CHE 2F04, CHE 2G03, CHE 3D04 (or concurrent)

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.

Required Textbook: Seider, Seader, Lewin, Widago, Ghani, Ming. "Product & Process Design Principles", 4th Edition, Wiley, 2016. E-book is cheap, especially US Amazon Kindle edition. Hardcopy has not yet been released yet and may not be in time for the course. The 3rd edition, including the international edition, is also ok to use. The 3rd edition hardcopy has an advantage because you can take it to open book exams. Book will be used in later courses too (4N04, 4W04)

Course Policies

Grading Policies

- Late submissions for take-home portions of exams will not be accepted w/o an MSAF.
- Valid MSAF forms for missed written midterms will result in **weight transferring** to the final. MSAFs for the in-lab midterm will result in a **retake**.
- Midterm and final exams will be **open book (any book) and open note**. In lab-exams have special restrictions on internet access.
- McMaster approved **calculators**, but not computers, may be used during the exams. However, it is unlikely you will need one.
- If technical difficulties prevent digital submissions to Ave2Learn, email it to a TA instead before the submission deadline.

Rules for Curving

Midterms, the project, & quizzes will not be curved. The final course grade will be curved in your favor as follows: x points will be added to your score, where $x = 95$ minus the **third highest score**. However x will never be larger than 10 or smaller than zero. Fractions of points will be rounded up. Final course percentage grades will be converted to **letter grades according to normal University policy**. I reserve the right to change the curve, but only in your favour and only in extreme circumstances.

Example: Priya got a 65.1 in the course. The top three students earned a 96, 94, and 91. Priya's curved course grade is $65.1 + (95 - 91) = 69.1\%$, rounds up to a 70%. This is reported as a B- to the registrar.

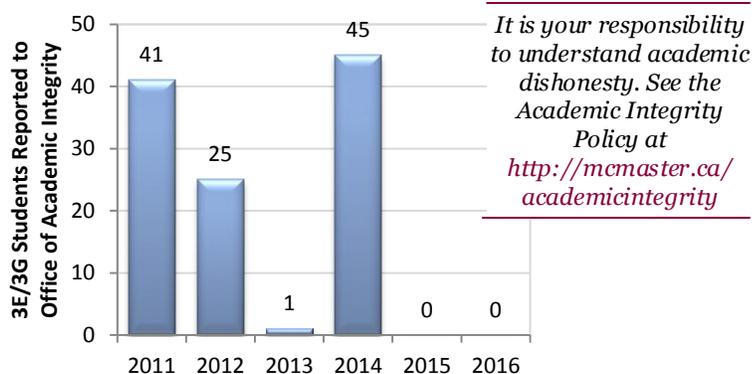
Grading Breakdown

Weight	Component	Comments
5%	Tutorials	11 tutorials – points for attendance .
40%	Midterms	10% + 10% + 20%. Details on later pages.
25%	Final Exam	2.5 hour written exam. Done individually.
5%	Quizzes	Short in-class online multiple choice quizzes (laptop or phone).
25%	Term Project	Includes graded milestone deliverables throughout the term. This is in place of graded homework. See next page for details.

Academic Honesty

- All marked quizzes and exams are to be done individually, with no collaboration with anyone. Midterm "re-takes" will be done in assigned groups.
- Tutorials and homework will not be marked. Feel free to work in groups or get outside help. It is for your understanding. If you work better alone, do it alone.
- 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.



Course Notes

Term Projects

Term projects will be completed in groups of up to five. **The project will be comprehensive and include everything learned in the course.** You will complete the project in stages over the course of the term by meeting the required project milestones (which will be graded).

You will be permitted to choose your own groups. If you are not part of a group I will assign you to a group. I may have to assign you to a group that has already formed. I have executive power to reassign and reform any group as I please, but I will only do this if the system is abused or if extreme circumstances warrant. I highly recommend you chose groups from within your tutorials so you can meet together during tutorial times.

The term projects will be partially delivered in the form of an oral examination with supporting materials such as simulation code, spreadsheets, calculations, and written deliverables. Points will be awarded for both technical accuracy as well as quality of the communication. Portions of the project will be delivered as "checkpoints" during the term.

The project will be related to synthesizing and analyzing a flowsheet which can be used to solve some chemical engineering problem. The results will be analyzed with regards to the triple-bottom-line of sustainability: cost, social impact, and environmental impact.

Previous sustainability-related topics by year:

2011: Synthesis of ethyl lactate, an environmentally friendly "green" solvent.

2012: Comparing the triple-bottom-line sustainability of coal and biomass to methanol processes, with and without CO₂ capture.

2013: Comparing the triple-bottom-line sustainability of chemical looping combustion to traditional natural gas combined cycles with CO₂ capture and sequestration.

2014: Biodiesel production from cooking oil wastes; Techno-economic and life cycle analysis.

2015: Dimethyl ether: a greener diesel substitute? Techno-economic and life cycle analysis.

2016: Greener plastics: Flare gas-to-olefins.

Term Project Grading

Milestones Portion 20%

Four milestone deliverables, worth 5% each, corresponding to the for course units. Think of these as homework.

Oral Exam, Group Portion 60%

Groups must defend their submission orally. This is not a presentation, but rather sitting down with me in my office and defending your work using evidence such as simulations, charts, tables, and the whatever deliverables have been assigned.

Oral Exam, Individual Portion: 20%

At the oral defence, you will be asked individual questions for individual credit.

Course Software

In this course, you will learn how to use chemical engineering software commonly used throughout the industry today. This will include:

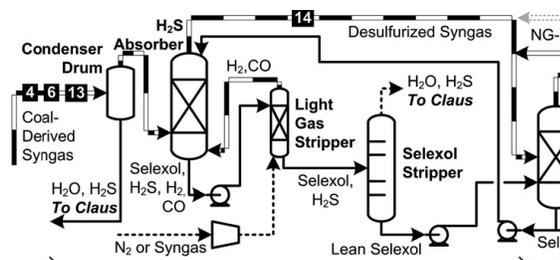
- **Aspen Plus:** A sequential-modular flowsheeting simulation program (EOR methods not covered) popular in the chemical and petrochemical industry. You are not required to purchase this software (you can't afford it!). It is available in all the UTS labs for free.
- **Aspen Capital Cost Estimator:** A program which computes very detailed capital cost estimates for chemical process equipment. Ditto, you will use this in the UTS Labs.
- **Aspen Energy Analyzer:** A program which creates an optimized heat exchanger network for your process. You will use this in the UTS Labs.
- **Open LCA:** An open source tool to compute life cycle inventories and life cycle impact analyses of chemical processes and their supply chains. You can get an open source version for free.
- And of course, office productivity software will also be used in this course for spreadsheeting and word processing. Feel free to use any version you like.

Note that lecture time will not focus on how to use these programs. Instead, this learning should take place during tutorials or during your homework and study time.

Course Calendar (subject to change!)

1. Basics of Process Flowsheets

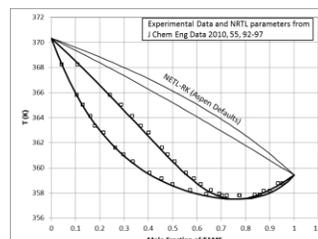
Reading, drawing, and understanding process flowsheets. We will also look at synthesising new flowsheets, handling steady states, recycles, escape routes, pressure-driven flows, and other key fundamentals.



Day	Topic	Read*	Quiz?
Jan 4	1.1: Course Intro		
Jan 5	1.2: Basic Concepts and Design Principles	Skills Test 1 Due Before Class	
Jan 9	1.2: Basic Concepts and Design Principles: Part 2	Ch 2 (4)	
Jan 11	1.3: Pressure Management	6.7, Ch 14 (20)	In Class
Jan 12	1.4: Temperature Skills Test Review	Skills Test 2 Due Before Class	
Jan 16, 18	1.4: Temperature Management	6.5, 6.6, 12.2(18.2)	In Class
Jan 19	1.5: Recycle/Purge/Waste & Other Design Heuristics	6.0-6.3	
Jan 23	1.6: Separation Heuristics	6.4, Ch 9(8)	In Class
Jan 25	1.7: Concept. Design Workshop	6.8-6.10	
Project Milestone 1: Due Feb 1		* 4 th Edition (Parenthesis is 3 rd Edition)	

2. Chemical Process Simulators

Common models and heuristics. Choosing the right models. Mathematical principles for solving systems of equations. DOF for physical properties and flowsheets. Sequential modular programs. Recycle, tears, and equation-of-state solvers.



Day	Topic	Read*	Quiz?
Jan 26	2.1: Common Physical Property Models		
Jan 30	2.2: Equation of State Models		
Feb 1	Midterm 1 – Individual Portion – T13/127 5:30PM – 7:20PM (extra hour)		
Feb 2	Midterm 1 – Group Retake		
Feb 6	2.3: Phase Equilibria		In Class
Feb 7	<i>Optional Project Milestone 1 Review & Help Session – JHE 210 12:30-1:20pm</i>		
Feb 8	2.4: Degree of Freedom Analyses and Flash Calculations		
Feb 9	2.5: Activity Coefficient Models		
Feb 13, 15	2.6: Stream, Mixer, and Heat Exchanger Models	12.2 (18.2)	In Class
Feb 16	2.7: Sequential Modular Flowsheeting	Ch 7 (5)	In Class
Project Milestone 2: Due March 1		* 4 th Edition (Parenthesis is 3 rd Edition)	

Tutorial Schedule (subject to change!)

Tutorial	Topic	T01	T02	T03
		Mo 2:30-4:20	Tu 9:30-11:20	We 9:30-11:20
Tutorial 1	Getting Started with Aspen Plus	Jan 9	Jan 10	Jan 11
Tutorial 2	Physical Property Modeling	Jan 16	Jan 17	Jan 18
Tutorial 3	Sensitivity Analysis and Design Spec	Jan 23	Jan 24	Jan 25
Tutorial 4	Utilities and Optimization	Jan 30	Jan 31	Feb 1
Tutorial 5	Advanced Reactor Models	Feb 6	Feb 7	Feb 8
Tutorial 6	Distillation Models	Feb 13	Feb 14	Feb 15
Tutorial 7	Calculator Blocks and Custom Models	Feb 27	Feb 28	Mar 1
Tutorial 8	Capital Cost Networks	Mar 6	Mar 7	Mar 8
Tutorial 9	Energy Analyzer / Heat Exchanger Networks	Mar 13	Mar 14	Mar 15
Tutorial 10	Advanced Distillation	Mar 20	Mar 21	Mar 22
Tutorial 11	Optional In-Lab Help – Projects and Midterm 3	Mar 27	Mar 28	Mar 29
Midterm 3	Covers all material to date–5:30-7:30p	Mar 29	Mar 29	Mar 29
Tutorial 12	OpenLCA and Life Cycle Analysis	Apr 3	April 4	April 5

Exam and Project Schedule (subject to change!)

Midterm 1 (10%)	Take Home Portion Assigned In-Class Portion Group-Portion (optional)	<i>Jan 30 – Due by in-class exam on Feb 2 Feb 1 Feb 2</i>
Midterm 2 (10%)	Take Home Portion Assigned In-Class Portion Group-Portion (optional).	<i>Feb 27 – Due by group exam on Mar 1 Feb 28 – T13 123 (A-O) T13-106 (P-Z) Mar 1</i>
Midterm 3 (20%)	In-Lab Only	<i>Mar 29 5:30p-7:30p</i>
Final Exam (25%)	As scheduled by registrar	<i>T1: JHE 233/234A T2: KTH – B121 T3: KTH – B123</i>
Term Project (25%)	Milestones 1 – 4 Project Deliverables Due Oral Exam Period	<i>See dates on previous pages Apr 6 Apr 10-21 – Scheduled with prof</i>

Note about Group-Portions of the Midterms

You will have the opportunity to submit a group copy of a midterm, done during the lecture period following a normal in-class individual midterm, handed in at the end of the 50 minute period. I reserve the right to choose groups. If the group grade is better than your individual grade, then your total, in-class midterm grade is weighted as 85% individual score, 15% group score. If your individual score is better, then your total midterm grade is 100% your individual grade. So there is no risk at all, it can only help you. There is no re-take associate with the take home portions. Students who miss the sitting (MSAF) are ineligible for the retake.

Learning Objectives

Key Learning Objectives and Topics

General Chemical Engineering Fundamentals

- 1st Law of Thermodynamics (Mass, Energy, Momentum Balances; Adiabatic vs exothermic vs endothermic)
- 2nd Law of Thermodynamics (Temperature crossover, pressure drop, entropy, exergy)
- Phase equilibria (VLE, VLLE, LLE).
- Fugacity, fugacity coefficients, activity coefficients, and models for phase equilibria.
- Chemical equilibria and associated models
- Sub-equilibrium reactions (Rate-based models)
- Degree of freedom analyses
- Thermodynamic state variables, how they relate, and how they can be modelled. (intrinsic vs extrinsic enthalpy, entropy, pressure, density, temperature, vapour fraction)
- Flash calculations (degrees of freedom, equations needed, phases needed, physical property models)

Conceptual Design Concepts

- Choosing correct temperature and pressure conditions for a process
- Choosing correct unit operations to achieve certain objectives and satisfy constraints
- Unit operations such as heat exchangers, valves, coolers, furnaces, flash drums, distillation, pumps, compressors, reactors, etc).
- Temperature and pressure management
- Use of recycle streams
- Use of purge streams
- Pressure-handling heuristics for turbines and compressors
- Heuristics for flash drums vs. distillation columns (which to choose?)
- Choosing between partial vapour partial-vapour-liquid, and total condensers
- Distillation synthesis for multi-component separation
- Identifying good candidates for separation
- Knowing how you would go about determining which of the candidates is best
- Reuse of valuable wastes (Steam cycles from waste heat, Fuel gases for furnaces or sale)

Aspen Plus

- What does each block do, what kind of unit operations can it model (there are typically more than one)?
- What are the model equations which are being solved under the hood?
- How do these model equations relate to mass, energy, momentum, phase, and summation balances? Are there any other thermodynamic properties or chemical engineering fundamentals that are used?
- What are the inputs to this model, what can you specify, what must you specify, and how many do you need to specify?
- What happens when I choose those particular inputs?
- What are the outputs of this model?
- When would I choose this model over other models? For example, Cyclone vs. SSplit, Heater vs HeatX, the different reactor types, the different separator types...
- Specific blocks: Mixer, FSplit, SSplit, Flash2, Flash3, Decanter, Sep, Heater, HeatX, DSTWU, Distl, RadFrac, Extract, Rstoic, RYield, REquil, RGibbs, RCSTR, RPlug, RBatch, Pump, Compr, MCompr, Valve, Mult, Dupl, Cyclone
- Tools such as: Design spec, Sensitivity, Calculator, and Optimization. (Why would I choose between these? What happens when you select something to output (Vary, Export, etc) which may overwrite the output of another program?)
- How do I pick good initial guesses (optimization, design spec)
- How do I pick good bounds on my variables? (Optimization, Design Spec, Sensitivity)
- Validating results (is it correct?)
- Tear streams, why we need them
- Computation order of sequential modular flowsheets
- Model a process in Aspen Plus, given a PFD Choosing the correct models and their correct inputs, Connecting the models together (which streams to I use and why), Creating models which improve convergence but have the same fidelity (e.g., using two Heater blocks instead of one HeatX, why we'd do that, and what we lose by doing that)
- Physical property models, and when to choose between them? (Is it always the same, how can you use data to help you choose, etc).

Learning Objectives

Key Learning Objectives and Topics Continued

Aspen Plus Continued

- Equation of state models – PR, SRK, Cubic EOS, phase roots to locate saturated vapour and saturated liquid points, Activity coefficient models – UNIQUAC, NRTL, UNIFAC, Tabular models - STEAMNBS)
- Physical property constants, parameters, database searches
- Property sets (See the activity coefficients of chemicals in a stream, fugacities, etc)
- Stream classes (MIXED, CISOLID, CIPSD, NCSOLID)
- Custom-defined molecules to use for UNIQUAC, UNIFAC estimation of molecules not contained in the database.
- Knowing when your results make sense or not
- Rate-based vs. Equilibrium-based modeling for distillation (and in general!)
- Data-Fit/Regression tools for getting reaction kinetics out of experimental data
- Utilities (how to implement in Aspen Plus, How to choose the correct ones, How to account for their costs (or sales!!! BFWLPS for example)
- Aspen Capital Cost Estimator (basic use, understanding how it links with Aspen Plus)
- Methods for best shot at convergence (Starting with simple blocks or strategies to get estimates, Gradually increase to more rigorous blocks using previous estimates as initial guesses to improve convergence, Using custom tear streams with initial guesses to improve convergence, Knowing when closing a recycle loop is important vs when we can keep it open (even if the real flowsheet definitely uses recycle), Getting better convergence by using good initial guesses for recycle streams without connecting the recycle stream at first.
- Understanding what Reinitializing really does
- Generating phase diagrams, bubble-dew point curves, etc.
- Understanding absolute vs. ratio-based modeling, i.e., is it ok if I choose some random basis for my scale? If so, is it easy to scale up later, and how would I do it? If I could choose between using reflux ratios, or reflux rates for a RadFrac spec, which ones would need to be changed if I were to scale it up?

Triple Bottom Line of Sustainability

1st Tier – Economics

- Six-tenths rule, Power law rules, Charts: cost vs size of unit, Using chemical engineering cost indices, Basic concepts of FOB purchase cost vs. Total direct cost, Utility costs
- Carbon Taxes
- Lifetime cost projections to compare different processes under different policies

2nd Tier – Environment

- Anything which is considered in this tier (resource depletion, climate change, water toxicity, human health, etc etc etc)
- Constructing a cradle-to-gate supply chain
- Life cycle inventories
- Incorporating Aspen Plus data
- Incorporating published data
- Performing yourself for simple systems
- Life cycle impact analyses
- Midpoint vs Endpoint methods
- IPCC 2007
- ReCiPe 2008 & EcoPoints
- Performing yourself for simple systems
- Elementary flows vs product flows
- Using OpenLCA
- Modeling a gate-to-gate process
- Inputs vs. Outputs
- Basis flows,
- Process basis and workaround for processes downstream of the process basis.
- Product systems
- General usability (knowing what output data mean, knowing how to type stuff in and where)

3rd Tier – Society

- 7 sins of greenwashing
- Knowing, being able to assess the greenness of actual commercial products.
- Conflicts of interest, conflicts with the other 2 tiers
- What kinds of things impact this tier (NIMBYs, noise, risk, emotions, etc)

Learning Objectives

...Continued

The Big Picture

Starting with a typical chemical engineering problem or objective (produce so much of X using these reaction pathways), can you:

- Propose one or more processes which can complete those objectives
 - Draw an annotated PFD that other engineers can read and understand
 - Identify when there is more than way to do something
 - Evaluate those processes in terms of the 1st (mass & energy & momentum) and 2nd (composition gradients, temperature gradients, pressure drop) laws of thermo by constructing models either by writing equations for the various steps involved or using software which has models of common process units already.
 - Simulate some or all of the process in Aspen Plus
 - Know which parts of the process need to be simulated, and how to best simulate it
 - Make and justify reasonable assumptions to make this happen.
 - Be able to interpret and understand the results.
- Run simulations to gather data using those models
 - Run the simulation under base case conditions
 - Rerun the simulation under different conditions or parameters
 - Perform sensitivity analyses or optimization to determine the best parameters to choose when the degrees of freedom are greater than 0.
 - Evaluate the process in terms of the triple bottom line
 - What is the cost/profitability of this process (in terms of dollars to the business)?
 - What is the (life cycle!) environmental impact of this process?
 - What are some social concerns raised by this process?
 - Make decisions and conclusions from these results
 - Should the company build or not build this process?
 - Is this process a better choice than other processes based on whatever criteria?
 - Will this process help, hurt, or potentially lessen the hurt to the environment?
 - Should government or businesses (or neither or both) invest certain technologies or processes based on your results?

CEAB Indicators & Outcomes

Indicator	Example Outcomes
Analysis: Ability to obtain substantiated conclusions as a result of a problem solution including recognizing the limitations of the solutions.	Make a critical assessment of model results to determine if the results have meaning, and if so, their level of accuracy
Tools: The ability to evaluate and select appropriate modern tools.	Employ Optimization, Sensitivity, and Design Spec blocks for advanced features in Aspen Plus
Ethics: Possesses the ability to apply ethical frameworks and reasoning in situations where there may be conflicting interests among the stakeholders.	Make assessments balancing the three tiers of the triple bottom line of sustainability, especially as it relates to shareholders (corporations, governments, and the people).
Impact: Assess possible options and design configurations from a sustainability engineering perspective, which emphasizes environmental stewardship, life-cycle analysis, and long-term decision-making principles.	Perform life cycle inventory and life cycle impact analyses using the ReCiPe method to determine environmental impacts and make suitable comparisons between processes
Economics: Understands the business processes for implementing engineering ideas.	Utilize the industry-standard Aspen Capital Cost Estimator software as a part of a profitability analysis.
Sustainability: Triple Bottom Line - An ability to design and evaluate complex open-ended engineering systems using a triple-bottom line of sustainability dimensions: social, economic and environmental.	Analyze and compare chemical processes based on profitability, social impact, and environmental impact.
Professionalism: Understands legal requirements governing engineering activities (including but not limited to personnel, health, safety, and risk issues)	Analyze the effect of carbon emission taxes or other environmental legislation on chemical plant design decisions or chemical plant operating decisions.