CHE 3G04 – CHEMICAL PROCESS SYNTHESIS AND SIMULATION

COURSE OUTLINE 2025

COURSE DETAILS

Instructor: Dr. Giancarlo Dalle Ave
dalleagf@mcmaster.ca

Teaching Assistants:

Lectures:

Tutorials:

Office Hours:

Prerequisites: ChE 2E04, ChE 2F04, ChE 3A04, ChE 3D04, ChE 3M04

McMaster University

DESCRIPTION

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

LEARNING OUTCOMES

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

- L1: 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.
- L2: Implement this flowsheet in a simulation program such as Aspen Plus.
- L3: Make use of thermophysical property models in the flowsheet. This includes identifying the correct models to use.
- L4: 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.
- L5: Construct custom models for unit operations which are not built into the software, and integrate them into the flowsheet.
- L6: Successfully run the flowsheet simulation to compute all mass and energy balances.
- L7: Extract useful information from the results and apply it towards the solving of the original problem.

▪L8: 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.

▪L9: Use the results of these flowsheet simulations to compute capital costs, energy costs, operation costs, and emissions to the environment.

▪L10: 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 STRUCTURE

COURSE BOOKS

1) Seider, *et. al*. "Product & Process Design Principles", 4th Edition, ISBN: 978-1-119-28263-1 (3rd edition works as well)
2) Adams II. "Learn Aspen Plus in 24 Hours", 2nd edition, ISBN: 9781264266654 (1st edition also works), Available online here (may have to access via university library website): https://www.accessengineeringlibrary.com/content/book/9781264266654

LECTURES

▪Lectures will be delivered live from BSB 119. Lectures will be recorded and posted online within 48 hours after the lecture (unless something goes wrong with the recording which happened before). Lectures will be posted to the course YouTube Playlist (link below).

▪Tutorials will be live in the computer lab and **attendance is required for marks** (in-tutorial assignments).

IF THE INSTRUCTOR CANNOT ATTEND

If for whatever reason I need to miss class I will as much notice as possible (difficult if I'm suddenly sick). If necessary, a recorded version of the lecture will be posted online to the YouTube playlist instead (link below).

COURSE POLICIES

COMPETENCY-BASED ASSESSMENTS

To support competency and self-efficacy, this course uses competency-based assessment; this form of assessment allows students to work on some aspects of a course individually, to achieve the required level of competency. Credit rather than a grade is given to those assessments. As in professional work, students are expected to demonstrate an acceptable level of competency for all CBA activities in order to pass the course.

There are three opportunities to demonstrate you have developed the required skills for each competency area. Activities must be completed to the standard required to pass for each activity. Activities cannot be skipped as they are how students demonstrate competency in the course learning outcomes.

It is up to you to demonstrate competency and contribution. It is not the TAs or Instructors role to demonstrate that you are not competent or that you did not contribute. Until you demonstrate you are competent in a learning outcome in/on an assessment - you are not considered competent.

The competencies evaluated in this course are:

C1: Chemical Engineering Design: Students must demonstrate that they are competent with the design principles discussed in this course. They must show that they can synthesize a flowsheet, which is thermodynamically feasible, not wasteful, and completes a given objective.

C2: Chemical Engineering Simulation: Students must demonstrate that they understand how to simulate a process using the discussed tools and that they understand the underlying principles upon which the simulators are built.

Each of these competencies will be assessed based on the following activities. Note that for midterm and final exam competency assessments there will be at least one question for each of the competencies. Questions which correspond to a competency assessment on the written midterm and the final exam will be clearly indicated.

Competency	Activity 1	Activity 2	Activity 3
C1 – Chemical Engineering Design	Design midterm question(s)	Design final exam question(s)	Final project individual interview
C2 – Chemical Engineering Simulation	Simulation written midterm question(s)	In-Lab Aspen midterm	Simulation final exam question(s)

GRADING AND MSAF POLICIES

Valid MSAF forms for missed written midterms, labs, or assignments 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, open note, and open device. All devices must be in airplane mode. If you're found to have a device not in airplane mode, you will automatically be given a zero on the exam. Any calculator may be used during the exams.

If technical difficulties prevent digital submissions to A2L, email it to a TA/the instructor instead before the submission deadline.

CURVING POLICY

Only final grades will be curved based on the instructor's discretion. The curve will never lower your grade, it can only improve it or leave it unchanged.

ACADEMIC DISHONESTY

All marked exams are to be done individually, with no collaboration with anyone. Collaboration is encouraged for assignments which can be completed in groups of up to three.

Tutorials will not be marked other than for completion. Feel free to work in groups. 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.

It is your responsibility to understand academic dishonesty. See the Academic Integrity Policy at http://mcmaster.ca/academicintegrity

GRADING BREAKDOWN

	Weight	Comment	Proposed Due Dates
Tutorials	10%	10 tutorials (completion marks) Note there are 11 tutorials scheduled meaning you can skip 1 and still get full marks or attend all 11 for a bonus mark.	Weekly
Midterms	35%	17.5% written + 17.5% Aspen midterms. More details on later pages.	Written: Feb 26th Aspen: Apr 3rd
Project	25%	Includes graded milestone deliverables throughout the term. More details on later pages.	1: January 26th 2: Feb 16th 3: March 16th 4: Apr 2nd (optional) Final Presentations: Week of April 7th
Final Exam	30%	2.5 hour written exam	TBD

COURSE NOTES

Note that all above due dates as well as the breakdown are subject to change. It is unlikely that major changes will occur but be sure to check on Avenue for minor changes to the grade breakdown and the due dates.

TERM PROJECT

Term projects will be completed in groups of four or 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 mainly for feedback purposes).

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 a presentation/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 milestones during the term. The purpose of the milestones will be to give you feedback on the project progress so that you have time to reevaluate design/simulation decisions going forward.

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.

TERM PROJECT GRADING

Milestones Portion 20%

Four milestone deliverables, worth 5% of the project each. Think of these as homework. The proposed due dates for the project deliverables are:

- Milestone 1: Process Design: January 26th
- Milestone 2: Process Simulation: Feb 16th
- Milestone 3: Process Optimization: March 16th
- Milestone 4 (optional): Economics + sustainability assessment: Apr 2nd

Presentation/Oral Exam, Group Portion 60%

The final project deliverable is a group presentation presenting key design and simulation decisions as well as a summary of results that will occur via Microsoft Teams. The presentations will occur the week of Apr 7th. An oral exam will follow in which groups must defend their submission and the decisions they made. Note that no design is ever perfect, part of the oral exam will focus on your ability to recognize things that could have been done better and discuss how you could go about changing them.

Presentation/Oral Exam, Individual Portion 20%

At the oral defence, I will call each individual group member into a breakout room. I will ask everyone questions about their design and the design process to assess their individual understanding of the material. This will be used to determine the individual portion of the project grade as well as the last portion of the Design Competency Based Assessment (please see above). The instructor reserves the right to adjust the weight of the group and individual components of the oral exams per individual at any time.

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 (equation oriented 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 and can be accessed either in the lab or using the Virtual Desktop service.
- **Aspen Capital Cost Estimator**: A program which computes very detailed capital cost estimates for chemical process equipment. Also available in the UTS Labs or via the Virtual Desktop service.
- **Aspen Energy Analyzer**: A program which creates an optimized heat exchanger network for your process. You can access this directly in the UTS labs or via the Virtual Desktop service.

MIDTERMS

The course will consist of two midterms. One written midterm and one in-lab midterm.

The written midterm will take place Wednesday February 26th from 6:30-8:30pm

The Aspen midterm will be a timed takehome midterm where you will be required to simulate a flowsheet in Aspen Plus. The midterm must be completed individually. The midterm will take place on Thursday April 3rd. You will have 24 hours to start and complete the midterm.

COURSE CALENDAR

The course is broken down into four major units:

- Unit 1: Process Flowsheeting: 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.

- Unit 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.

- Unit 3: Unit Operation Modeling: Equilibrium, Gibbs, extent of reaction, and kinetic reactor models. Flash drums, distillation, stripping, and rectification. Equilibrium and rate-based distillation.

- Unit 4: Triple Bottom Line of Sustainability: Using software for equipment costing and economics. Operating costs, utilities, feed costs, raw materials, labour, and energy costs. Life cycle analyses, society impacts, responsibilities. Using software to determine the sustainability of chemical processes and supply chains.

An approximate course calendar can be found in the table on the next page (which subject to change depending on how fast I talk in class).

Week	Date	Unit	Lecture Topic	Tutorial	Assigned	Due	Book Chapters
1	Jan 6th	1-1	Intro	1 - Getting started with Aspen Plus	Project group formation		Ch 2 (4)
		1-2	Design Principles				
		1-3	Design and Pressure			Project group formation	
2	Jan 13th	1-4	Temperature management	2 – Physical Property Modeling	Project milestone 1		Ch 6.5-6.7, 12.2 (18.2), 14 (20)
		1-5	Recycles, purges, waste				
		1-6	Separation heuristics				
3	Jan 20th	1	Review	3 – Problem Solving Tools	Project milestone 2		Ch 6-6.4, 6.8-6.10, 9 (8)
		1-7	Conceptual design workshop				
		2-1	Thermophysical property models			Project milestone 1	
4	Jan 27th	2-2	EoS models	4 – Heat Exchangers			Ch 12.2 (18.2)
		2-3	Phase equilibria				
		2-4	Flash calculation + DoF				
5	Feb 3rd	2-5	Activity coefficient models	5 – Equilibrium-Based Distillation Models			
		2-6	HeatX and Split Models				
		2-7	Sequential Modular Flowsheeting				
6	Feb 10th	2	Review	6 – Advanced Problem Solving Skills	Project milestone 3		
		1+2	Written Midterm Review				
			Catch-up day			Project milestone 2	
7	Feb 24th	3-1	Rstoic and Ryield	7 – Chemical Reactor Models			Ch 7 (5), 15.2 (N/A)
		3-2	Equilibrium models			Written midterm	
		3-3	Kinetic Reaction Models				
8	March 3rd	3-4	HeatX Networks	9 – Custom Models + External Control			Ch 11-11.4 (9-9.4)
		3-5	Shortcut distillation models				
		3-6	Equilibrium distillation models				
9	March 10th	3	Review	11 – Heat Exchanger Networks			Ch 13-13.5 (19-19.5
		1+2	Written midterm take up				
		4-1	Intro to sustainability		Project milestone 4	Project milestone 3	
10	March 17th	4-2	Costs and economics	8 -Rate-Based Distillation			Ch 3.3-3.5 (N/A) 16 (22)
		4-2	Capital Costs				
		4-3	Operating Costs				
11	March 24th	4-4	LCA Boundaries	10 – Capital Cost Estimation		Project milestone 4 (optional)	
		4-5	LCI				
		4-6	LCIA				
12	March 31st	4-7	Social Impacts	Aspen Midterm Week			
		4	Review			In-Lab (Aspen) midterm	
		All	Exam Review				
13	Apr 7th		Catch-up day			Project presentations	

Note: dates presented in the course outline are approximate only. Please pay attention to announcements in-class and on A2l for up-to-date information.

TUTORIALS

Tutorials in this class will be in-lab where you will gain first hand experience of the software in the course. These tutorials will be marked for completion (they have to be correct to get the full marks). The tutorial instructions are very detailed so following them directly should enable you to easily complete the tutorials.

We will be covering the tutorials in a different order than the textbook. The TAs are aware of this, but please ensure you complete the right tutorial in any given week. To avoid any confusion, the tutorial activities are also presented in the approximate course calendar given above. The number in the table corresponds to the "Tutorial Activity Number" in the second edition textbook. Please make sure to complete the correct tutorial for each week.

OFFICE HOURS

Office hours with both the instructor and the TAs are by appointment only. This is subject to change as later in the course an official office hours section may open for project help.

To book office hours with the instructor, please use the following link:

If you are unable to find a suitable time via the bookings link, please email the instructor directly to setup a time. Meetings will be either in-person or online depending on the instructor's availability.

To book office hours with the TAs, please contact them and arrange a time/place directly.

IMPORTANT LINKS

Please find below a list of important links for the class. They'll be mentioned throughout the term but a comprehensive list follows:

If you're unable to find a lot via the bookings link, please email me to arrange a time. Meetings with be online or in-person depending on my availability.

Instructor/TA Emails:

Instructor:

Giancarlo Dalle Ave: dalleagf@mcmaster.ca

OTHER/MISC.

THE P.R.O.C.E.S.S.

The department of Chemical Engineering has a storied history of education. In addition to teaching and learning, the department is proud of our graduates not only for their academic success, but their more intrinsic traits that make them respected members of the engineering community.

Recently, several high-ranking graduates from the McMaster Chemical Engineering Program employed in various industries (oil/gas, financials, etc.) were interviewed to ask what traits they look for when hiring for engineering positions. Using this information, the department would like to present to you the PROCESS: a code of conduct that we hope will guide our students throughout this program and their careers to come.

- **P**rofessionalism
- **R**esponsibility
- **O**wnership
- **C**uriosity
- **E**mpathy
- **S**elflessness
- **S**ervice

It is up to YOU to interpret these traits and apply them to your time at McMaster and your career as you see fit. These traits will not be assessed for grades but will be strongly encouraged throughout your time at McMaster. We hope that you identify with these character traits and what they mean to you, and that you trust the process.

INCLUSIVE ENVIRONMENT

Everyone in our teaching team considers the classroom to be a place where you will be treated with respect, and we welcome individuals of all ages, backgrounds, beliefs, ethnicities, genders, gender identities, gender expressions, national origins, religious affiliations, sexual orientations, ability – and other visible and non-visible differences. All members of the class are expected to contribute to a respectful, welcoming, and inclusive environment for every other member of the class. We will gladly honour your request to address you by an alternate name or gender pronoun. Please advise us of this preference early in the semester.

COPYRIGHT AND RECORDINGS

Students are advised that lectures, demonstrations, performances, and any other course material provided by an instructor include copyright protected works. The Copyright Act and copyright law protect every original literary, dramatic, musical and artistic work, including lectures by University instructors.

The recording of lectures, tutorials, or other methods of instruction may occur during a course. Recording may be done by either the instructor for the purpose of authorized distribution, or by a student for the purpose of personal study. Students should be aware that their voice and/or image may be recorded by others during the class. Please speak with the instructor if this is a concern for you.

ACADEMIC ACCOMMODATIONS FOR RELIGIOUS, INDIGENOUS, OR SPIRITUAL OBSERVANCES

Students requiring academic accommodation based on religious, indigenous or spiritual observances should follow the procedures set out in the RISO policy. Students should submit their request to their Faculty Office normally within 10 working days of the beginning of term in which they anticipate a need for accommodation or to the Registrar's Office prior to their examinations. Students should also contact their instructors as soon as possible to make alternative arrangements for classes, assignments, and tests.

C.E.A.B. GRADUATE ATTRIBUTES

Certain courses in the chemical engineering curriculum collect indicator data related to the development of the attributes deemed critical for engineers according to the Canadian Engineering Accreditation Board (CEAB). These indicators (detailed at the beginning of the outline) will be assessed throughout the course and redacted samples of student work may be collected for submission to the CEAB during McMaster Engineering's accreditation cycle. The indicators assessed in ChE 3G04 are as follows:

1.4 – Competence in mathematics.

4.3 – Competence in engineering fundamentals.

4.4 – Evaluates engineering tools, identifies their limitations, and selects, adapts, or extends them appropriately.

5.2 – Successfully uses engineering tools.

9.1 – Demonstrates comprehension of technical and non-technical instructions and questions.

11.1 – Applies economic principles in decision making

Indicator	Mapped Learning Outcomes
1.4	L1, L3, L4
4.3	L2, L4, L5
4.4	L7
5.2	L5, L6, L8
9.1	L 9, L10
11.1	L9, L10

The CEAB indicators listed above are mapped to the course learning outcomes as shown in the following table. The CEAB accreditation process is an important component to curriculum design in engineering. If you have any questions or wish to be involved in the accreditation process, please let me know at dalleagf@mcmaster.ca.