CHEMENG 3D04 Chemical Engineering Thermodynamics

Course Outline – Fall 2025

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In case of conflicts, the latest version of this document posted on the course's A2L page prevails.

TEACHING STAFF

Role	Name	E-mail	Office Hours
Instructor	Li Xi	xili@mcmaster.ca	Announced on A2L
Teaching Assistants	TA1	–	TBD
	TA2	–	
	TA3	–	

Getting your questions answered

- Office hours all follow an open-door policy, meaning that all students are welcome to join the conversation and no privacy should be expected. This applies to in-person, online, and hybrid formats
- Regularly held office hours may be cancelled or changed to a different format with prior notice.
- Generally, the instructor will answer conceptual questions about course contents, while the TAs will assist you with computer labs and assignments.

SCHEDULE

Day(s)	Time*	Calendar Designation	Our Designation
Tue	11:30–12:20	C01	1hr Class Sessions
Thu	10:30–12:20		2hr Class Sessions
Mon	14:30–16:20	T02	Computer Labs
Tue	14:30–16:20	T01	
Thu	14:30–16:20	T03	

*Per university policy, class venues are not listed in the course outline. Check your Mosaic account for venue information.

TEXTBOOK

Required

[S&VN-9] J. M. Smith, H. C. Van Ness, M. M. Abbott, and M. T. Swihart, *Introduction to Chemical Engineering Thermodynamics*, 9th Edn., McGraw-Hill, 2022

Notes:

- Alternative versions of the book, such as earlier editions and international editions, are acceptable. It is the student's responsibility to address any gaps between editions.
- Written exams in the course allow the use of the textbook, but only formally published hard copies will be accepted. Electronic copies and their printouts, or photocopies, will not be allowed. **It is the student's responsibility to ensure that a hard copy of the textbook is available for exams.**
- Exam policies put a limit on the amount of notes that a student can bring. It is the student's responsibility to ensure that their textbook is free of substantial notes or writings. (Simple markups, such as highlights, single words or short phrases, are acceptable.)

COMMUNICATION

Avenue to Learn (http://avenue.mcmaster.ca/; also referred to as "Avenue" or "A2L") will host the main course webpages, where course materials, documents, assignments, online discussion, important announcements, and other related information will be posted/hosted. The students are expected to check the course A2L page regularly.

McMaster E-mail Account The "@mcmaster.ca" E-mail accounts will also be used for course-related correspondence. The students are expected to check their E-mail accounts regularly. (Note: A2L has its separate *internal E-mail system*, which *will NOT be used or checked*.)

Microsoft Teams (https://teams.microsoft.com/; also referred to as "MS Teams" or just "Teams") will be used for additional class-related communications, including online meetings and direct messages. The students are expected to log in regularly to their Teams accounts associated with their MacIDs and be able to receive messages there.

COURSE OBJECTIVES

This course discusses the fundamental theories of thermodynamics and their application in chemical engineering processes, with particular focuses on non-ideal and multicomponent systems and on thermodynamic equilibrium analysis. Students are expected to grasp the following knowledge:

Theoretical Framework definitions of thermodynamic properties and the mathematical relations therebetween, especially for non-ideal fluids and mixtures;

Thermodynamic Models material-specific models for thermodynamic properties, including models for non-ideal fluids and non-ideal mixtures, and their connections with experimental data;

Equilibrium Analysis the concept of thermodynamic equilibrium and criteria for its determination, with applications in phase and chemical reaction equilibria.

After the course, students should also be able to set up mathematical formulations for thermodynamic problems, understand the assumptions behind the mathematical models and equations, and solve the equations using analytical and numerical approaches.

OUTLINE OF TOPICS*

1. Introduction
   - Thermodynamics and chemical engineering
   - Basic concepts and laws of thermodynamics: a brief review
   - A math refresher
2. Thermodynamic Properties and Relations
   - PVT behaviors and equation of state
   - Free energy and property relations
   - Residual properties
3. Vapor-Liquid Equilibrium (VLE)
   - Equilibrium criteria and one-component VLE
   - Raoult's law and multicomponent VLE calculations
   - VLE of general mixtures: Pxy behaviors and models
4. Solution Theory – Thermodynamic Properties of Mixtures
   - Partial properties and chemical potential
   - Ideal-gas mixture
   - Fugacity
   - Ideal solution
   - Non-ideal solutions: activity and excess properties
5. Thermodynamics of Mixtures and Mixing

- Multicomponent VLE and models for the activity coefficient
- Phase separation and equilibria
- Mixing: property changes and heat effects

6. Chemical Reaction Equilibrium
   - Introduction: stoichiometry and equilibrium criterion
   - Evaluation of the equilibrium constant
   - Single-reaction equilibrium in homogeneous systems
   - Multi-reaction equilibrium in homogeneous systems
   - Reaction equilibrium in heterogeneous systems

*Subject to change at the instructor's discretion.

METHOD OF DELIVERY

The course adopts a "flipped classroom" format with the following elements.

Lectures (online/pre-recorded) Students are required to watch online lecture videos before corresponding contents are further discussed in the class. A schedule of the assigned videos for every week will be posted on A2L.

Quizzes (online) Quizzes of short questions must be completed on A2L after watching the lecture recordings.

Class Sessions Class sessions will be in-person and are designed to help the students consolidate their learned knowledge from recorded lectures. Activities may include brief summaries of online videos, Q&A about lecture contents, example problems, and in-class exercises.

Computer Labs The course contains a computer lab component where numerical methods are used to solve thermodynamic problems. Computer lab sessions are organized around numerical problems, each of which will take 1 to 2 sessions to complete. Instructions will be given in Matlab®, but students are also allowed to complete the assigned tasks in Python if they so choose.

Assignments Take-home problems will be assigned on A2L, to be submitted approximately on a bi-weekly basis.

ASSESSMENT PROCEDURE

Term Grade Calculation

The term percentage grade of each student will be calculated with both Schemes A and B. The higher result will be recorded as the original, *as-calculated* term grade of the student.

Category	Num.	Schedule/Due	Scheme	
			A	B
Quizzes	11	23:59 on Mondays.	5%	5%
Assignments	5	as indicated on A2L.	5%	5%
Computer Lab Reports	5	as indicated on A2L.	20%	20%
Midterm Exams	2	(1) Oct. 2 and (2) Nov. 13; 10:30 – 12:20.	40%	0%
Final Exam	1	to be scheduled.	30%	70%

- The instructor reserves the right to change the number and format of each assessment item.
- Assignments and computer-lab reports must be submitted electronically to corresponding A2L assignment folders. *Submission through unauthorized channels (MS Teams, E-mail, etc.) will be ignored.*
- The due day for computer lab reports is the same for different computer lab sessions.

- Weight of each individual quiz or assignment in the corresponding category is proportional to the number of graded questions in that quiz/assignment.

Passing Criteria and Grade Reporting

In addition to receiving an as-calculated term grade that is *no less than* 50/100, the student must also satisfy **one of the following two conditions** to pass the course.

1. Final exam grade is *no less than* 50/100; ***OR***
2. Final exam grade is lower than 50 but *no less than* 40/100, ***and*** the average of midterm grades is *no less than* 50/100.

For students who meet the criteria above, their as-calculated term grades will be converted to letter grades using the Registrar's recommended procedure. For students who fail to meet the criteria above, a grade of "F" will be assigned (regardless of their as-calculated grade value).

Grade adjustment may be applied at the instructor's discretion.

Missed Work Policies

- Unless otherwise noted, relief for missed work must be requested through the McMaster Student Absence Form (MSAF) system.
- *The onus is on the student to contact the instructor* for missed work relief after completing the MSAF process.
- Specific grading procedures for missed work with valid MSAF requests are provided below for each assessment category.
- A zero mark will be given for missed work without MSAF.

Lecture Quizzes

- The quizzes are graded for completeness only.
- During the entire term, each student is allowed to have *up to 3 late submissions with no mark loss*. Such late submissions must be received ***within 7 calendar days*** from the original deadline. MSAF is not required for these late submissions.
- Extension beyond this 7-day limit and additional late submissions will both require valid MASF.
- Missed submissions will receive zero marks.

Assignments

- Assignments are graded for completeness only. Reasonable attempts at solving the problems will receive full marks. Lack of serious efforts will be given zero marks.
- With a valid MSAF, reasonable extension may be granted. Such extension requests must be submitted before the original deadline. Requests received after the original deadline will not be considered unless justification acceptable to the instructor is provided.
- Without MSAF, each late submission is subject to a penalty of 1% for every hour late (rounded to the next whole hour).

Computer Lab Reports

- Computer lab reports will be graded for both completeness and correctness.
- With a valid MSAF, reasonable extension may be granted. Such extension requests must be submitted before the original deadline. Requests received after the original deadline will not be considered unless justification acceptable to the instructor is provided.
- The report requirement may be waived, with its weight moved to the final exam, if extension is not possible at the time when the MSAF is received, under the constraint that **each student cannot waive more than two reports over the entire term**.
- Without MSAF, each late submission is subject to a penalty of 1% for every hour late (rounded to the next whole hour).

Midterm Exams

- Two 110 min midterm written exams are scheduled.
- With a valid MSAF, the weight of the missed exam will be moved to the final exam.

Final Exam

- The final exam will be a written exam.
- The coverage will be comprehensive, including contents of the whole course.
- MSAF does not apply to the final exam. Please refer to McMaster's deferred examination policies.

ADDITIONAL POLICIES ON ASSESSMENT

Aids Allowed in Written Exams

The **one book + one sheet rule** will be followed in all written exams. Students will be allowed to bring:

- a *formally published* hard copy of the designated textbook: i.e., S&VN*;
- one sheet of **hand-written** notes (letter size, double-sided; print-outs or photocopies are not allowed);
- any calculator;
- writing/drawing tools;
- timepiece (with no computing or communication functions).

No other books or materials will be allowed. Electronic devices not in the list will be forbidden, including but not limited to computers, tablets, cell phones, smart watches, PDAs, and any other devices with computing or communication capabilities. Any evidence of violation will be treated as a case of academic dishonesty.

*Annotations in the form of individual words, symbols, short phrases, and short expressions are allowed in the textbook; extended notes – long or multiple sentences, paragraphs, groups of equations, etc. – are prohibited.

Use of Generative AI

Students may use generative AI, *for computer-lab reports only,* in either of the following ways

- brainstorming and polishing their languages to more clearly convey the student's own ideas and thought processes, and
- learning programming/coding techniques by using generative AI to generate a template or example code which the student may modify and adapt to their own needs.

Generative AI cannot be used to replace the student in intellectually analyzing the problem, constructing a solution path, completing mathematical derivation and calculation, and critically analyzing the results. All submitted work must reflect the student's own original thinking.

Any instance of using generative AI, such as each sentence or code generated, must be clearly referenced and declared, in a reference list at the end of the document. For example,

> *The sentence/code starting from [. . .] to [. . .] on page [. . .] was originally generated by ChatGPT 3.5 [or any other version or AI tool that you used] and revised by myself [or] used as is.*

If generative AI was not used, the following statement is required at the end of the submitted document:

> *I declare that the submitted report is entirely my original intellectual work. Generative AI tools have not be used in its preparation.*

It is the student's responsibility to be clear on the limitations for use and to be clear on the expectations for citation and reference and to do so appropriately. Use of generative AI outside the above guidelines, in any other assessment items, or without proper reference/declaration will constitute academic dishonesty.

It is also expected that *generative AI tools will only be used sporadically* as an aid to the student's learning process. Excessive use, i.e., when a substantial portion of the work was generated by AI, can lead to mark deduction due to the lack of a serious effort.

Other Aids, Collaboration, and Academic Integrity

For *quizzes*, *assignments*, and *computer lab reports*:

- Students are encouraged to discuss with each other, but each student must submit their own work.
- With the exception of objective questions (e.g., multiple choice), identical or unreasonably similar answers will be considered an act of plagiarism or improper collaboration.

For *written exams*:

- Students will only be allowed to use the aids specified on the exam paper.
- Communication with others, including *but not limited to* other students, either in person or remotely (through telephone, messaging, internet, or any other electronic communication method) is strictly prohibited.

For all categories of assessment, academic integrity infractions *will be reported to the Academic Integrity Office*, in addition to heavy penalties on the grade.

Additional Screening of Computer Lab Reports

- At the discretion of the instructor, an arbitrary number of submitted computer lab reports will be subject to additional screening for academic integrity compliance.
- The instructor may call on selected students for oral examination. The examination is not intended as an additional assessment step for grading purpose. It is instead designed to test their knowledge of the submitted work.
- Signs of improper collaboration or reliance on AI or other aids that exceeds the boundary of the above policies, as reflected by the student's inadequate knowledge of their own work and its underlying thought process, will be treated as ***a case of academic dishonesty***.

Grade Challenge

To challenge the grading of an graded item (*other than the final exam*), the following procedure must be followed.

- A written request must be sent to

  d-ChE3DTeaching@mcmaster.ca

- The request needs to contain a detailed list of the alleged grading errors, with page/line numbers specified (as appropriate) and reasons/justifications provided.
- The student is responsible for submitting a copy of the graded material along with the request.
- The instructor and/or TAs will review the request and may call for meetings with the student if further discussion is needed.

The graded *final exam* may be reviewed upon written request *to the instructor* (through @mcmaster.ca E-mail accounts). Its re-grading, if requested, is subject to the following conditions.

- It may only be re-graded if there is sufficient evidence of major mistakes in the original grading that have substantially affected the outcome.
- Once started, the final exam will always be regraded in its entirety – *the new grade may be lower than the original*.

Partial Credit

- Partial credit may be awarded for incorrect answers at the discretion of the instructor or TAs.
- Accumulation of errors: if an incorrect answer of one step is partially or fully caused by incorrect answer(s) from previous steps, partial credit will only be assigned for correct conceptual understanding/thought process as reflected in the written solution. The instructor/TAs will not check whether the calculation process of the new step itself is correct by attempting to reproduce the answer from the wrong results of previous steps.

Accreditation Information

Learning Outcomes of the Course

1. Understand the definitions and roles of thermodynamic properties in pure fluids and mixtures.
2. Understand the mathematical framework connecting different thermodynamic properties. Learn to derive unknown properties from known ones.
3. Understand idealized model systems, such as ideal gas and ideal solution, including their underlying assumptions. Understand the departure of real fluids and mixtures from idealized models.
4. Understand the applicability of thermodynamic models for fluid and mixture properties. Be able to obtain model parameters from experimentally measurable quantities.
5. Understand the concept of thermodynamic equilibrium and the criteria for its identification from thermodynamic properties.
6. Understand the application of thermodynamics principles to chemical processes, especially phase equilibrium and chemical reaction equilibrium.
7. Understand the application of mixture thermodynamics to fluid mixing and phase separation.
8. Develop the capability of formulating mathematical problems for equilibrium and heat analysis of chemical processes. Understand the assumption(s) behind the chosen solution path. Be able to solve such problems using appropriate mathematical procedures.
9. Acquire the experience of applying engineering computing software to solve complex thermodynamic problems, use basic numerical methods, such as numerical differentiation and integration, to evaluate thermodynamic relations, and use regression and data visualization to critically analyze the numerical solution.

CEAB Indicators Associated with the Course

The following information is required by the Canadian Engineering Accreditation Board (CEAB). Graduating from an accredited institution has many advantages. Detailed information is found at http://www.engineerscanada.ca/accreditation.

No.	CEAB Indicator	Learning Outcomes
1.1	Competence in Mathematics	L.O. 2, 8, and 9
1.3	Competence in Engineering Fundamentals	L.O. 1, 2, 3, and 5
1.4	Competence in Specialized Engineering knowledge	L.O. 4, 6, and 7
2.1	Identifies and states reasonable assumptions and suitable engineering fundamentals, before proposing a solution path to a problem.	L.O. 3 and 8
5.2	Successfully uses engineering tools.	L.O. 9

The P.R.O.C.E.S.S.

As some of you may already be aware, 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.

- Professionalism
- Responsibility

- Ownership
- Curiosity
- Empathy
- Selflessness
- Service

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**.

APPROVED ADVISORY STATEMENTS

The following statements are required per McMaster's Undergraduate Course Management Policies.

Academic Integrity

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. **It is your responsibility to understand what constitutes academic dishonesty.**

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. For information on the various types of academic dishonesty please refer to the Academic Integrity Policy, located at https://secretariat.mcmaster.ca/university-policies-proceduresguidelines/.

The following illustrates only three forms of academic dishonesty:

1. plagiarism, e.g. the submission of work that is not one's own or for which other credit has been obtained.
2. improper collaboration in group work.
3. copying or using unauthorized aids in tests and examinations.

Authenticity/Plagiarism Detection

Some courses may use a web-based service (Turnitin.com) to reveal authenticity and ownership of student submitted work. For courses using such software, students will be expected to submit their work electronically either directly to Turnitin.com or via an online learning platform (e.g. A2L, etc.) using plagiarism detection (a service supported by Turnitin.com so it can be checked for academic dishonesty.

Students who do not wish their work to be submitted through the plagiarism detection software must inform the Instructor before the assignment is due. No penalty will be assigned to a student who does not submit work to the plagiarism detection software. **All submitted work is subject to normal verification that standards of academic integrity have been upheld** (e.g., on-line search, other software, etc.). For more details about McMaster's use of Turnitin.com please go to www.mcmaster.ca/academicintegrity.

Courses with an On-Line Element

Some courses may use on-line elements (e.g. e-mail, Avenue to Learn (A2L), LearnLink, web pages, capa, Moodle, ThinkingCap, etc.). Students should be aware that, when they access the electronic components of a course using these elements, private information such as first and last names, user names for the McMaster e-mail accounts, and program affiliation may become apparent to all other students in the same course. The available information is dependent on the technology used. Continuation in a course that uses on-line elements will be deemed consent to this disclosure. If you have any questions or concerns about such disclosure please discuss this with the course instructor.

Online Proctoring

Some courses may use online proctoring software for tests and exams. This software may require students to turn on their video camera, present identification, monitor and record their computer activities, and/or lock/restrict their browser or other applications/software during tests or exams. This software may be required to be installed before the test/exam begins.

Conduct Expectations

As a McMaster student, you have the right to experience, and the responsibility to demonstrate, respectful and dignified interactions within all of our living, learning and working communities. These expectations are described in the Code of Student Rights & Responsibilities (the "Code"). All students share the responsibility of maintaining a positive environment for the academic and personal growth of all McMaster community members, **whether in person or online**.

It is essential that students be mindful of their interactions online, as the Code remains in effect in virtual learning environments. The Code applies to any interactions that adversely affect, disrupt, or interfere with reasonable participation in University activities. Student disruptions or behaviours that interfere with university functions on online platforms (e.g. use of Avenue 2 Learn, WebEx or Zoom for delivery), will be taken very seriously and will be investigated. Outcomes may include restriction or removal of the involved students' access to these platforms.

Academic Accommodation of Students with Disabilities

Students with disabilities who require academic accommodation must contact Student Accessibility Services (SAS) at 905-525-9140 ext. 28652 or sas@mcmaster.ca to make arrangements with a Program Coordinator. For further information, consult McMaster University's Academic Accommodation of Students with Disabilities policy.

Requests for Relief for Missed Academic Term Work

In the event of an absence for medical or other reasons, students should review and follow the Policy on Requests for Relief for Missed Academic Term Work.

Academic Accommodation for Religious, Indigenous or Spiritual Observances (RISO)

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.

Copyright and Recording

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.

Extreme Circumstances

The University reserves the right to change the dates and deadlines for any or all courses in extreme circumstances (e.g., severe weather, labour disruptions, etc.). Changes will be communicated through regular McMaster communication channels, such as McMaster Daily News, A2L and/or McMaster email.