ChE 3D04 Chemical Engineering Thermodynamics

Course Outline – Fall 2021

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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	by appointment
Teaching Assistants	Arniel Ching Dizon	dizona3@mcmaster.ca	1:30 – 3:20 pm, Fridays
	Song Yi (Dawn) Lin	lins70@mcmaster.ca	
	Juan Doratt Mendoza	dorattj@mcmaster.ca	
	Naveen Vasudevan	vasudevn@mcmaster.ca	

Office Hours

- The instructor offers *flexible* office hours on an as-needed basis. *E-mail appointment in advance is required.* His availability can be found through his McMaster Outlook calender.

  https://xiresearch.org/lx-calendar/

- Office hours are delivered through MS Teams by default. If in-person meetings are requested, please confirm with the TA for availability.
- Students are encouraged to use the "Discussions" page on A2L, where the instructor/TAs will check regularly to answer questions.

SCHEDULE

Day(s)	Time	Venue		Calendar Designation	Our Designation
		In-Person	Virtual		
Tue, Thu, Fri	11:30–12:20	N/A	MS Teams	C01	Class Meetings
Tue	08:30–10:20	BSB 244	MS Teams	T01	Computer Lab
Wed	10:30–12:20	BSB 249	MS Teams	T02	Computer Lab

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 (obtain from the Campus Store).

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.

Microsoft Teams (https://teams.microsoft.com/; also referred to as "MS Teams" or just "Teams") will host all virtual meetings related to the course (unless otherwise announced), including regular class meetings, computer lab sessions (virtual attendance option), and office hours.

Important documents and information, such as class notes and real-time announcements during class sessions or remote exams, will also be shared via MS Teams. The students are required to remain members of the class Team

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and their corresponding tutorial/computer lab session Team

CHEMENG 3D04 T01 FAL 2021 Chemical Engineering Thermodynamics

or

CHEMENG 3D04 T02 FAL 2021 Chemical Engineering Thermodynamics

during the offering and check messages there 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*.)

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) Pre-recorded lectures must be watched before class meetings according to the schedule posted on A2L.

Quizzes (online) A quiz of short questions must be completed on A2L after watching all assigned lecture videos of the week.

Practice Problems (online) These problems are designed to prepare the students for answering long, often calculation-based, questions in exams and should be completed by the students after watching corresponding lecture videos. They used to belong to assignments in previous offerings but now submission is no longer required and they are no longer graded. Instead, solutions are provided for the students to study at their own pace.

Class Meetings (virtual/live) The three scheduled class sessions of each week will be used to help consolidate students' learning outcomes and address problems arising from the online learning process. *Attendance is NOT required and is at the students' discretion.* In a typical week, the sessions are allocated as follows.

Tue	summary of recorded lectures and review of the quiz.
Thu	open office hour.
Fri	example problem(s) and discussion.

Note: this arrangement is subject to change during the term.

Computer Lab (in-person or virtual/live) The course contains a computer lab component where numerical computation with Matlab® is used to solve thermodynamic problems. Each computer lab session will focus on an assignment which the students will submit for grading. Computer lab sessions are offered in person (as long as it is permitted by University policies and public health guidelines), but an option of virtual attendance will be provided.

ASSESSMENT PROCEDURES

Grading Schemes

Category	Schedule/Due	Scheme	
		A	B
Lecture Quizzes	11:59 pm, the following Monday	5%	5%
Computer Lab Assignments	(preliminary/25%) one hour after the session end	25%	25%

	(final/75%) 11:59 pm, the following Monday		
Midterm Exams	evenings of (1) Oct. 7 and (2) Nov. 11	40%	0%
Final Exam	to be scheduled	30%	70%

- Unless otherwise specified, all items are submitted to A2L. *Submission through unauthorized channels (MS Teams, E-mail, etc.) will be ignored.*
- **To pass the course, the student must receive at least 35% of the marks in the final exam.**
- The student's term grade will then be calculated with either scheme A or scheme B, whichever gives a higher result.
- Adjustment/re-curving of the term grade may be applied at the discretion of the instructor.
- The final letter grade will be assigned using the Registrar's recommended procedure.

Missed Work Policies

- 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.
- Each student is *allowed to miss up to 2 quizzes*, without having to use MSAF, during the entire term while still retaining full marks.
- With a valid MSAF, reasonable extension will be granted for completing the specified quiz.
- Late submission without MSAF *will NOT be accepted*.

Computer Lab Assignments

- *The preliminary submission does NOT have to be complete* and it will only be graded for participation. Its purpose is to compel the students to get as much finished as possible during the session. Reasonable progress will receive full marks, while clear lack of participation or inadequate efforts will be penalized.
- The final submission will be graded for both completeness and correctness.
- With a valid MSAF, reasonable extension will be granted. The assignment requirement may be waived, with its weight move 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 such assignments over the entire term**.
- Without MSAF, late preliminary submission *will NOT be accepted* and late final submission is subject to a penalty of 1% for every hour late (rounded to the next whole hour).

Midterm Exams

- Two two-hour midterm evening exams are scheduled.
- With a valid MSAF, the weight of the missed exam will be moved to the final exam.
- In case of online exams, late submission without MSAF is subject to a lateness penalty (see below).

Final 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.

- In case of an online exam, late submission is subject to a lateness penalty.

Lateness Penalty for Online Exams

In the event that any exam (midterm or final) is arranged online, lateness penalty is calculated as follows.

- A base value of 10% penalty is *always applied for any late submission*.
- *Plus,* an additional penalty of 1% is added for each minute late (rounded to the next whole minute).

For example, if your submission is $1\,\mathrm{min}$ and $15\,\mathrm{s}$ late, which will be rounded up to $2\,\mathrm{min}$, the lateness penalty will be $10\% + 2\% = 12\%$.

Important Note: it is the responsibility of the student to ensure that they have adequate technical hardware and software and internet connection to complete the submission on time and to budget time for potential equipment or internet glitches. The instructor does not have the knowledge, expertise, or capability to verify claims of equipment or internet malfunction and thus will not make exceptions for such circumstances. *The receipt time recorded on A2L will be the only accepted time stamp for submission.*

ADDITIONAL POLICIES ON ASSESSMENT

Collaboration, Aids, and Academic Integrity

For *lecture quizzes* and *computer lab assignments*:

- 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 *midterm exams* and the *final exam*:

- 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.

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 the instructor* (through @mcmaster.ca E-mail accounts).
- 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 policies.

- 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 graded in its entirety – *the new grade may be lower than the original*.

Partial Credit

- In tests and exams, partial credit may be awarded for incorrect answers at the discretion of the instructor and 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. Note: 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

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.

1. Competence in Mathematics.
2. Ability to identify reasonable assumptions (including identification of uncertainties and imprecise information) that could or should be made before a solution path is proposed.
3. Capable of selecting appropriate models and methods and identify assumptions and constraints.

Learning Outcomes of the Course

	Learning Outcomes	CEAB Indicators
•	Understand the definitions and physical meanings of various thermodynamic properties for both pure fluids and mixtures.	1
•	Understand the mathematical framework connecting different thermodynamic properties.	1
•	Understand the concepts of and assumptions behind idealized model systems such as ideal gas and ideal solution.	2, 3
•	Understand the departure of real fluids, including mixtures, from idealized models and be able to select and utilize appropriate models to describe real fluids, including models for their PVT behaviors and activity coefficients.	1, 2, 3
•	Understand the concept of thermodynamic equilibrium and the criteria for its identification from thermodynamic properties.	1
•	Be able to select the appropriate model to analyze a given vapor-liquid equilibrium (VLE) system and understand its connections with the general equilibrium criteria.	1, 2, 3
•	Understand the miscibility and phase separation of multiple liquids and be able to analyze the heat effects and equilibrium composition of their mixing.	1, 3
•	Understand the concept of and criteria for chemical reaction equilibrium and be able to analyze the equilibrium composition of both homogeneous and heterogeneous reactive mixtures.	1, 2, 3
•	Be able to solve thermodynamic equilibrium analysis problems, using analytical and/or numerical approaches as appropriate.	1
•	Be able to apply thermodynamic property relations to calculate thermodynamic properties of fluids and materials from experimentally measurable quantities, using analytical and/or numerical approaches as appropriate.	1, 3

• Be able to extract parameters for thermodynamic models from experimental data by combining statistical analysis with numerical computation.	1, 2, 3

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**.

STATUTORY 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 Expectation

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

McMaster Student Absence Form (MSAF): In the event of an absence for medical or other reasons, students should review and follow the Academic Regulation in the Undergraduate Calendar "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.