# ChE 3D04 Chemical Engineering Thermodynamics

## Course Outline – Fall 2023

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*Department of Chemical Engineering, McMaster University*

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

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## TEACHING STAFF

| Role | Name | E-mail | Office Hours |
|------|------|--------|--------------|
| Instructor | Li Xi | xili@mcmaster.ca | by appointment |
| Teaching Assistants | Arniel Ching Dizon | dizona3@mcmaster.ca | TBD |
| | Hana Mirvakili | mirvakin@mcmaster.ca | |
| | Youdi Zhang | zhang125@mcmaster.ca | |

### Getting your questions answered

- The instructor offers *flexible* office hours on an as-needed basis. *E-mail appointment in advance is required.* Please propose at least two time options and indicate whether you prefer an in-person or online meeting. His availability can be found through his McMaster Outlook calender.
- The TAs will hold regular office hours specifically to address questions about take-home and computer-lab assignments.
- Students are encouraged to use the "Discussions" page on A2L as an online office-hour room, where the instructor/TAs will check regularly to answer questions.

## SCHEDULE

| Day(s) | Time* | Calendar Designation | Our Designation |
|--------|-------|---------------------|-----------------|
| Mon, Wed | 11:30–12:20 | C01 | Class Meetings |
| Fri | 13:30–14:30 | | |
| Thu | 12:30–14:20 | T01 | Computer Lab |
| Fri | 10:30–12:20 | T02 | Computer Lab |

*Per university policy, venues for class sessions cannot be listed in the course outline. Check your Mosaic account or the course A2L page.

## 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).
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.
- 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.
- 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 keep an active Teams account 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

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*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)** Before each class meetings, students are required to watch the corresponding lecture recordings as assigned on A2L.

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

**Class Meetings** Class meetings will be used to help the students consolidate their learned knowledge from recorded lectures. Activities may include brief recaps of lecture contents, examples, class discussions, and in-class exercises.

**Computer Labs** The course contains a computer lab component where numerical computation with Matlab® is used to solve thermodynamic problems. Computer lab sessions are organized around numerical problems, each of which will take 1 to 2 sessions to complete.

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

## ASSESSMENT PROCEDURES

### Grading Schemes

| Category | Num. | Schedule/Due | Scheme | |
|---|---|---|---|---|
| | | | A | B |
| Lecture Quizzes | $\sim 30$ | 11:59 pm, the day before class | 5% | 5% |
| Take-Home Assignments | $\sim 6$ | as indicated at A2L | 5% | 5% |
| Computer Lab Assignments | $\sim 6$ | as indicated at A2L | 20% | 20% |
| Midterm Exams | 2 | evenings of (1) Oct. 5 and (2) Nov. 9 | 40% | 0% |
| Final Exam | 1 | to be scheduled | 30% | 70% |

- The instructor reserves the right to change the number and format of the assessment methods.
- Take-home and computer-lab assignments must be submitted electronically to corresponding A2L assignment folders. *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.
- During the entire term, each student is allowed to have *up to 8 late submissions (without using MSAF) with no mark loss*. Such late submissions must be received within 7 calendar days from the original deadline.
- With a valid MSAF, additional extension may be granted.
- Missed submissions will receive zero marks.

### Take-Home Assignments

- Take-home 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.
- Without MSAF, each late submission is subject to a penalty of 1% for every hour late (rounded to the next whole hour).

### Computer Lab Assignments

- Computer lab assignments will be graded for both completeness and correctness.
- With a valid MSAF, reasonable extension may be granted.
- The assignment 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 such assignments 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 two-hour midterm evening exams are scheduled.
- With a valid MSAF, the weight of the missed exam will be moved to the final exam.

### 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.

## ADDITIONAL POLICIES ON ASSESSMENT

### Aids Allowed in Test/Exam

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

- a *formally published* hard copy of the designated textbook: i.e., S&VN\*;
- one sheet of notes (letter or A4 size, double-sided; must be **hand-written**, printed or photocopied copies 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.

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*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 assignments 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 assignment 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 generative by AI, can lead to mark deduction due to the lack of a serious effort.

### Other Aids, Collaboration, and Academic Integrity

For *lecture quizzes*, *take-home assignments*, 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

    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 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

- 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. 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

### 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.