

# ChE 3D04 Chemical Engineering Thermodynamics

## Course Outline – Fall 2020

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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
Instructor	Li Xi	<a href="mailto:xili@mcmaster.ca">xili@mcmaster.ca</a>
Teaching Assistants	Song Yi (Dawn) Lin	<a href="mailto:lins70@mcmaster.ca">lins70@mcmaster.ca</a>
	Naveen Vasudevan	<a href="mailto:vasudevn@mcmaster.ca">vasudevn@mcmaster.ca</a>
	Ziqi (Zeke) Gao	<a href="mailto:gaoz24@mcmaster.ca">gaoz24@mcmaster.ca</a>

### Office Hours

- The instructor and TAs offer *flexible* office hours on an as-needed basis. *E-mail appointment in advance is required.*
- The instructor's availability can be found through his McMaster Outlook calendar.

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

- Students are encouraged to use the “Discussions” page on A2L, where the instructor/TAs will check regularly to answer questions.
- Additional office hours and/or town-hall style Q&A sessions may be offered, usually before exams or major due dates.

### SCHEDULE AND DELIVERY

Day(s)	Time	Location	Calendar Designation	Our Designation
Tue, Thu, Fri	11:30–12:20	MS Teams	C01	In-Class Discussion
Tue	08:30–10:20	MS Teams	T01	Tutorial/Computer Lab
Thu	08:30–10:20	MS Teams	T02	Tutorial/Computer Lab

- The course will adopt a “flipped classroom” format.
- Students are asked to watch prerecorded lectures before classes, according to the schedule posted on A2L.
- The scheduled class hours (session C01) will be used for in-class discussions and short assignments (e.g., conceptual questions, short calculations).
- The scheduled tutorials (session T01 or\* T02) will be used for more in-depth assignments, including both paper-and-pencil calculations/derivations and numerical computation.
- Numerical computation will be performed with Matlab® which all McMaster students are licensed to use. To install, follow the instruction below.  
<https://www.mathworks.com/academia/tah-portal/mcmaster-university-31501097.html>.
- Additional practice problems may be posted on A2L, which are not graded but may help with exam/test preparation.

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\*Identical contents will be covered between T01 and T02.

## TEXTBOOK

### **Required**

[S&VN-8] J. M. Smith, H. C. Van Ness, M. M. Abbott, and M. T. Swihart, *Introduction to Chemical Engineering Thermodynamics*, 8th Edn.\*, McGraw-Hill, 2018

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\*The 7th edition is also 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.

**Microsoft Teams** (<https://teams.microsoft.com/>; also referred to as “MS Teams” or just “Teams”) will host all class-related meetings (unless otherwise announced), including regular class meetings, tutorials/computer lab sessions, Q&A sessions, and office hours. Students are *required to log in with their MacID* and use the code

**tg472q7**

to join the “ChE3D04 Fall 2020” Team.

**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.

## 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.

## ASSESSMENT PROCEDURES

### Grading Schemes

Category	Schedule/Due	Scheme	
		A	B
Lecture Quizzes	11:59 pm the day before the class (schedule on A2L)	5%	5%
In-Class Assignments	during the class	5%	5%
Tutorial Assignments	individually specified due dates	20%	10%
Monthly Tests	evenings of (1) Sep. 30, (2) Oct. 28, and (3) Nov. 25	40%	20%
Final Exam	to be scheduled	30%	60%

- 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 40% 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

- Students are required to watch prerecorded lectures and complete their attached quizzes, by 11:59 pm of the night before the corresponding class sessions (see schedule on A2L).
- These assignments are graded for completeness only.

- Each student is allowed to miss up to 10% of the assignments in this category to retain full marks.
- With a valid MSAF, reasonable extension will be granted for completing the specified assignment(s).
- Late submission without MSAF will NOT be accepted.

### **In-Class Assignments**

- These assignments are completed during the regular class hours (session C01) and submitted during the class.
- These assignments are graded for completeness only.
- Each student is allowed to miss up to 20% of the assignments in this category to retain full marks.
- With a valid MSAF, the student will be allowed to make up for the missed assignment(s). They are required to contact the instructor for appointment for this purpose.
- Late submission without MSAF will NOT be accepted.

### **Tutorial Assignments**

- Part of these assignments are to be completed during the tutorial sessions and the rest are take-home.
- The tutorial and take-home parts will be submitted as a whole by the due date specified for each assignment.
- With a valid MSAF, either reasonable extension will be granted or the weight will be moved to the final exam. The choice between the two options is at the discretion of the instructor.
- Late submission without MSAF is subject to penalty (1% for every hour late, rounded to the next whole hour).

### **Monthly Tests**

- A total of 3 tests are scheduled in the evening of the last Wednesday of each month.
- Each test is designed for the duration of one hour.
- For each student, the lowest test grade of the three will be discarded. The average of the remaining test grades is counted for this category.
- With a valid MSAF, the weight of the missed test will be moved to the final exam.
- Late submission without MSAF is subject to penalty (to be specified on the test paper or at A2L).

### **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.
- Late submission is subject to penalty (to be specified on the exam paper or at A2L).

## **ADDITIONAL POLICIES ON ASSESSMENT**

### **Collaboration, Aids, and Academic Integrity**

For *lecture quizzes, in-class assignments, and tutorial 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 *monthly tests* and the *final exam*:

- Tests and exams are open book and open notes.

- Other allowed aids will be specified for each test/exam.
- 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**

<b>Learning Outcomes</b>	<b>CEAB Indicators</b>
<ul style="list-style-type: none"> <li>• Understand the definitions and physical meanings of various thermodynamic properties for both pure fluids and mixtures.</li> </ul>	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 <i>PVT</i> 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

## 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](https://secretariat.mcmaster.ca/university-policies-proceduresguidelines/), 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](https://www.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](https://www.turnitin.com) or via an online learning platform (e.g. A2L, etc.) using plagiarism detection (a service supported by [Turnitin.com](https://www.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](https://www.turnitin.com) please go to [www.mcmaster.ca/academicintegrity](http://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](mailto: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

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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.