ChE 3D03 Chemical Engineering Thermodynamics

Course Outline – Fall 2017

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August 24, 2017*

This is a preliminary release of the course outline for your information only. The formal outline of the course will be updated on its Avenue page and the latest version posted there always supersedes this or any other earlier versions.

1 General Information

• INSTRUCTOR

Li Xi
Office : JHE-345/C
Extension : 27020
E-mail : xili@mcmaster.ca
Office hour : [TBD] or by appointment*.

*Subject to change or cancellation upon prior notice. Additional office hours may be arranged before tests/exams.

• TEACHING ASSISTANTS

Name	E-mail	Office Hour	Room
Sahar Samani	esmaeils@mcmaster.ca	[TBD]	[TBD]
Naveen Vasudevan	vasudevn@mcmaster.ca	[TBD]	[TBD]
Kurt Westhaver	westhavk@mcmaster.ca	[TBD]	[TBD]

• CLASS SCHEDULING

Time	Room	Calendar Designation	Our Designation *
Mon 17:30–18:20	MDCL-1309	C01	Lecture
Wed 17:30–18:20	MDCL-1309	C01	Lecture
Thu 15:30–16:20	MDCL-1110	T01	Tutorial (or Lecture†)
Thu 17:30–18:20	MDCL-1309	C01	Lecture

*Designation of class slots is subject to change upon prior notice.
†The tutorial slot may occasionally be used for lectures upon prior notice.

• TEXTBOOK

– Required –

[S&VN] J. M. Smith, H. C. Van Ness, and M. M. Abbott, *Introduction to Chemical Engineering Thermodynamics*, 7th Edn., McGraw-Hill, 2005

• COMMUNICATION

Important information, announcements, and course materials will be posted on the "Avenue to Learn" website (http://avenue.mcmaster.ca/). The "@mcmaster.ca" E-mail accounts (of the instructor, TAs, and students) will be used for course-related correspondence. The onus is on the students to check their

*Future revisions of this document posted on the course Avenue page will always supersede earlier versions.

"Avenue" and "@mcmaster.ca" E-mail accounts regularly. (**Important:** do NOT use the internal E-mail system of the "Avenue".)

2 Course Contents

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[a]

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
   - Mixing: property changes and heat effects
   - Phase separation and equilibria

[a] Subject to change at the instructor's discretion.

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

3 Assessment Procedures

Grading Scheme

Assessment Items	Schedule (when; where)	Scheme	
		A	B
Assignments	approximately biweekly; dropbox outside JHE-374	10%	10%
Midterm Test 1 (120mins)	Oct. 3 (Tue.) 19:00–21:00; MDCL-1105	25%	0%
Midterm Test 2 (120mins)	Nov. 7 (Tue.) 19:00–21:00; MDCL-1105	25%	0%
Final Exam (150mins)*	TBA by the Registrar's Office	40%	90%

*Required for a passing grade.

- The final exam will be comprehensive. **Important**: writing the final exam is required for passing the course.
- The term percentage grade will be determined with the scheme giving higher score for each student.
- 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

- Weight of missed work (assignments/tests) with a valid MSAF request will be transferred to the final exam.
- A zero mark will be given for missed work without any MSAF.

Assignment Policies

- Each student must submit his/her own solutions. Identical or close-to-identical solutions will be penalized (usually zero mark) and the infraction will be reported to the Academic Integrity Office.
- The student's name and student number must be on the top of each page.
- Due date/time will be specified for each assignment. Late submission will not be accepted unless prior approval is granted by the instructor (before the deadline).
- Each assignment problem will be graded in a scale of 0–2, according to the following rubric.

Grade	Meaning
2	The answer is correct, largely correct, OR at least demonstrating a substantial effort in the correct direction.
1	The answer is marginally satisfactory with significant errors, missing components, or deviation from the correct solution path. However, it shows a considerable effort that is relevant to the question.
0	No response, irrelevant answers, or no serious effort demonstrated.

Important: Getting a score of 2 does not mean that the answer is correct; the students are still responsible for checking their answers using the solution posted. The assignment problems are an important resource for test/exam prepration.

Test/Exam Policies – Aids Allowed
The **one book + one sheet rule** will be followed in all tests/exams. Specifically, 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.

*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.

Test/Exam Policies – Grading and Partial Credit

- Partial credit maybe awarded for correct approaches or steps even when the final answer is wrong.
- Distribution of partial marks is at the discretion of the instructor.
- If a wrong answer is obtained at one step, the student automatically loses all the partial marks attributed to calculation in all following steps that depend on that wrong number; however, he/she may still be entitled to the partial marks for the concepts or solution approaches if they are correct.

Policies and Procedure for Re-grading/Re-marking Requests

- **Important**: Assignments/Tests/Exams must be written in permanent ink to be eligible for re-grading. Grading of materials written in pencil will be final and cannot be challenged.

Re-grading requests (final exam excluded) must be submitted according to the following procedure:

- Re-grading requests must be made within 14 calendar days (weekends/holidays included) after the graded material is first available for pick-up and no later than the final exam date (whichever is earlier).
- The student must send (through E-mail) a written request for re-grading to the instructor, listing all places where the original grading is challenged (with the problem and page numbers specified) and provide justification for each request.
- The original material must be handed in to the instructor or TAs within 7 calendar days after the written request.
- The instructor/TAs may call for meetings with the student to further discuss the re-grading request.

4 Accreditation Information

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.

CEAB Indicators Associated with the Course

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	Corresponding 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

5 Statutory Statements

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."

"Academic dishonesty is to knowingly act or fail to act in a way that results or could result in unearned academic credit or advantage. This behaviour can result in serious consequences, e.g. the grade of zero on an assignment, loss of credit with a notation on the transcript (notation reads: 'Grade of F assigned for academic dishonesty'), and/or suspension or expulsion from the university."

"It is your responsibility to understand what constitutes academic dishonesty. For information on the various types of academic dishonesty please refer to the Academic Integrity Policy, located at http://www.mcmaster.ca/academicintegrity/.

"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."

Use of "Avenue to Learn"

In this course we will be using the "Avenue to Learn" website. "Students should be aware that, when they access the electronic components of this course, 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 this course will be deemed consent to this disclosure." If you have any questions or concerns about such disclosure please discuss this with the course instructor.

Academic Accommodation of Students with Disabilities

"Students who require academic accommodation must contact Student Accessibility Services (SAS) to make arrangements with a Program Coordinator. Academic accommodations must be arranged for each term of study. Student Accessibility Services can be contacted by phone 905-525-9140 ext. 28652 or e-mail sas@mcmaster.ca. For further information, consult McMaster University's Policy for Academic Accommodation of Students with Disabilities."

The Faculty of Engineering Policies

"The Faculty of Engineering is concerned with ensuring an environment that is free of all adverse discrimination. If there is a problem, that cannot be resolved by discussion among the persons concerned, individuals are reminded that they should contact the Department Chair, the Sexual Harassment Officer or the Human Rights Consultant, as soon as possible."