NANYANG TECHNOLOGICAL UNIVERSITY SINGAPORE

COURSE CONTENT

Academic Year	2023/2024	**Semester**	2
Course Coordinator	Asst. Prof. Tej Salil Choksi / Dr. Poernomo Gunawan		
Course Code	CH2123		
Course Title	Chemical Thermodynamics		
Pre-requisites	CH1104 Materials & Energy Balances, CB1117 Engineering Mathematics, CH1108/CH2108 Thermodynamics		
No of AUs	3		
Contact Hours	26 hours lecture, 12 hours tutorial		
Proposal Date	4 Oct 2021		

Course Aims

This course aims to teach you thermodynamics at a more advanced level, to study thermodynamics concepts and principles in relation to open flow systems, ideal and non-ideal gas and liquid mixtures, and to apply them on chemical engineering processes, in particular, thermodynamics cycles, liquefaction, phase equilibria and chemical equilibria.

Intended Learning Outcomes (ILO)

Upon completion of the course, you should be able to:

1. Apply the laws of thermodynamics to develop and evaluate the performance of thermodynamics cycles.
2. Develop and derive mathematical correlations among thermodynamics properties for ideal and non-ideal gas and liquid mixtures.
3. Apply thermodynamics principles of mixtures/solutions on phase and chemical equilibria.

Course Content

1. Review of basic laws and concepts of thermodynamics;
2. Joule-Thompson effect, thermodynamics efficiencies of turbine, pump, and compressors;
3. Thermodynamics analysis and interpretation of phase diagrams;
4. Thermodynamic analysis of refrigeration, gas liquefaction, and Rankine cycle;
5. Partial molar properties, chemical potential and concept of fugacity;
6. Thermodynamics principles of ideal and non-ideal gas mixtures: residual properties, Gibbs-Duhem theorem, and fugacity coefficient;
7. Thermodynamics principles of ideal and non-ideal solution: excess properties, Lewis-Randal rule, and activity coefficient;
8. Phase equilibria: Raoult's law and modified Raoult's law, bubble points and dew points calculations;
9. Chemical reaction equilibria.

Assessment (includes both continuous and summative assessment)

Component	Course LO Tested	Related Programme LO or Graduate Attributes	Weighting	Team /Individual	Assessment rubrics
Continuous Assessment: Quiz #1	1	EAB-SLO a), b), c)	20%	Individual	Appendix 1
Continuous Assessment: Quiz #2	2,3	EAB-SLO a), b), c)	20%	Individual	Appendix 1
Continuous Assessment: Class Participation #1	1	EAB-SLO a), b), c), d)	5%	Individual	Appendix 2
Continuous Assessment: Class Participation #2	2,3	EAB-SLO a), b), c), d)	5%	Individual	Appendix 2
Final examinations (2 hours, Open Book, exam paper not allowed to be removed from exam hall)	1, 2, 3	EAB-SLO a), b), c)	50%	Individual	Appendix 1
Total			100%		

Mapping of Course ILOs to EAB Graduate Attributes

Course Intended Learning Outcomes	Cat	EAB's 12 Graduate Attributes*											
		(a)	(b)	(c)	(d)	(e)	(f)	(g)	(h)	(i)	(j)	(k)	(l)
	Core	●	●	●	◐								

Apply the laws of thermodynamics to develop and evaluate the performance of thermodynamics cycles	a, b, c
Develop and derive mathematical correlations among thermodynamics properties for ideal and non-ideal gas and liquid mixtures	a, b, c
Apply thermodynamics principles of mixtures/solutions on phase and chemical equilibria	a, b, c, d

Legend:
- ● Fully consistent (contributes to more than 75% of Intended Learning Outcomes)
- ◐ Partially consistent (contributes to about 50% of Intended Learning Outcomes)
- š Weakly consistent (contributes to about 25% of Intended Learning Outcomes)
- Blank Not related to Student Learning Outcomes

Formative feedback

a) Feedback for the assignment will be returned to the students.
b) After each quiz, the solutions will be posted on NTUlearn and students are welcome to set a consultation to address their doubts and misconception.

Learning and Teaching approach

Approach	How does this approach support students in achieving the learning outcomes?
Lecture	Lectures would primarily discuss the fundamentals and concepts of

	thermodynamics, as well as demonstrate the procedures of deriving and solving mathematical equations.
Tutorial	Tutorial questions comprise relevant applications of the concepts introduced in lectures. Students are encouraged to have discussion with the instructor to clarify doubts and to explore cases beyond the tutorial questions.

Reading and References

1) Smith J.M., Van Ness H C and Abbott MM, "Introduction of Chemical Engineering Thermodynamics", McGraw Hill, 7th Edition in SI Units (2005)
2) S. I. Sandler, “Chemical and Engineering Thermodynamics”, 2nd Edition, Wiley, (2001).
3) J.R. Elliot and C.T. Lira, “Introductory Chemical Engineering Thermodynamics”, 1st edition, Prentice Hall PTR, (1999).

Course Policies and Student Responsibilities

General: You are expected to complete all online activities and take all scheduled assignments and tests by due dates. You are expected to take responsibility to follow up with course notes, assignments and course related announcements. You are expected to participate in all tutorial discussions and activities.

Continuous assessments: You are required to attend all continuous assessments. The continuous assessments have two components, weekly polls, and a homework. Both the polls and homework are graded with respect to completion and not for correct/wrong answers. These assessments are meant to help you stay up to date with what is going on every week,

Absenteeism: Continuous assessments make up a significant portion of students’ course grade. Absence from continuous assessments without officially approved leave will result in no marks and affect your’ overall course grade.

Academic Integrity

Good academic work depends on honesty and ethical behaviour. The quality of your work as a student relies on adhering to the principles of academic integrity and to the NTU Honour Code, a set of values shared by the whole university community. Truth, Trust and Justice are at the core of NTU’s shared values.

As a student, it is important that you recognize your responsibilities in understanding and applying the principles of academic integrity in all the work you do at NTU. Not knowing what is involved in maintaining academic integrity does not excuse academic dishonesty. You need to actively equip yourself with strategies to avoid all forms of academic dishonesty, including plagiarism, academic fraud, collusion and cheating. If you are uncertain of the definitions of any of these terms, you should go to the academic integrity website for more information. Consult your instructor(s) if you need any clarification about the requirements of academic integrity in the course.

Course Instructors

Instructor	Office Location	Phone	Email
Tej Salil Choksi	N1.2-B1-18	63168940	tej.choksi@ntu.edu.sg
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Planned Weekly Schedule

Week	Topic	Course LO	Readings/ Activities
1	Review of the first and second laws of thermodynamics	1	Smith Van Ness Chapters 1, 2, 5
2	Ideal work, irreversible work, Joule-Thompson effect, thermodynamics analysis of turbine, pump, and compressors.	1	Smith Van Ness Chapters 5, 7
3	Non-adiabatic turbines/compressors, irreversible processes, flashing	1	Smith Van Ness Chapters 5, 7
4	Thermodynamic analysis of Rankine cycle.	1	Smith Van Ness Chapter 8
5	Thermodynamic analysis of refrigeration cycles	1	Smith Van Ness Chapter 9
6	Thermodynamic analysis of gas liquefaction processes	1	Smith Van Ness Chapter 9
7	Partial molar properties, Gibbs-Duhem theorem.	2	Smith Van Ness Chapter 11
8	Chemical potential and concept of fugacity.	2	Smith Van Ness Chapter 11
9	Thermodynamics analysis of ideal and non-ideal gas mixtures: residual properties, Gibbs-Duhem theorem, and fugacity coefficient.	2	Smith Van Ness Chapter 11
10	Thermodynamics analysis of ideal and non-ideal solution: excess properties, Lewis-Randall rule, and activity coefficient.	2	Smith Van Ness Chapter 11
11	Activity coefficient models (Margules, Van Laar, NRTL), phase equilibria (Raoult's law, modified Raoult's law).	2	Smith Van Ness Chapter 12
12	Thermodynamics analysis of chemical equilibria: reaction coordinate, heat of reaction and Gibbs free energy of	3	Smith Van Ness Chapter 13

	reaction.		
13	Thermodynamics analysis of chemical equilibria: equilibrium constant, vant Hoff equation, Le Chatelier principle.	3	Smith Van Ness Chapter 13

Appendix 1: Assessment Criteria for Quiz and Final Examination

Criteria	Unsatisfactory: <40%	Borderline: 40% to 49%	Satisfactory: 50% to 69%	Very good: 70% to 89%	Exemplary: >90%
Develop and evaluate the performance of thermodynamics cycles	Unable to formulate the problem, unable to construct and evaluate the efficiencies of basic thermodynamics cycles and do not know how to use and interpret thermodynamics phase diagrams (P-H, T-S, P-V diagrams)	Able to formulate the problem, able to interpret thermodynamics phase diagrams but having difficulty to construct and evaluate the efficiencies of basic thermodynamics cycles.	Able to formulate the problem, able to interpret thermodynamics phase diagrams and to use them to construct and evaluate the efficiencies of basic thermodynamics cycles.	Able to formulate the problem, able to interpret thermodynamics phase diagrams and to use them to construct and evaluate the efficiencies of complex thermodynamics cycles.	Excellent understanding of the problem, good interpretation of thermodynamics phase diagrams and able to translate complex thermodynamics cycles on multiple phase diagrams
Develop mathematical correlations among thermodynamics properties for ideal and non-ideal gas and liquid mixtures	Unable to formulate the problem, unable to identify which thermodynamics properties are involved and do not know how to develop appropriate mathematical thermodynamics equations to solve the problems.	Able to formulate the problem and to identify which thermodynamics properties are involved but do not know how to develop mathematical thermodynamics equations to solve the problems.	Able to formulate the problem and to identify which thermodynamics properties are involved, able to write their mathematical relationships.	Able to formulate the problem and to identify which thermodynamics properties are involved, able to use their mathematical relationship correctly to solve mixing problems.	Good understanding of the problem and the correlations among thermodynamics properties, know their limitations and how to combine with materials & energy balances to solve complex mixing problems.
Apply thermodynamics principles of mixtures/ solutions on phase equilibria	Unable to apply the concepts of phase equilibria to construct phase equilibrium diagram; unable to calculate bubble and dew points for ideal and non-ideal mixtures, and do not know how to correctly interpret the phase equilibrium diagram.	Able to apply the concepts of phase equilibria to construct phase equilibrium diagram for ideal mixtures; know how to correctly interpret the diagram, but having difficulty in calculating bubble and dew points for ideal mixtures.	Able to apply the concepts of phase equilibria to construct phase equilibrium diagram for ideal mixtures; know how to correctly interpret the diagram as well as to calculate bubble and dew points for ideal mixtures.	Able to apply the concepts of phase equilibria to construct phase equilibrium diagram for ideal and non-ideal mixtures; know how to correctly interpret the diagram as well as to calculate bubble and dew points for ideal and non-ideal mixtures.	Excellent understanding of phase equilibrium for ideal and non-ideal mixtures, including homogeneous and heterogeneous azeotropes.
Apply thermodynamics principles on chemical equilibria	Unable to determine correlations between thermodynamics properties and equilibrium constant; unable to set up mathematical equations to solve for equilibrium compositions and reaction coordinate.	Able to determine correlations between thermodynamics properties and equilibrium constant but having difficulty to write mathematical equations to solve for equilibrium compositions and reaction coordinate.	Able to determine correlations between thermodynamics properties and equilibrium constant and able to develop mathematical equations to solve for equilibrium compositions and reaction coordinate for single reaction.	Able to determine correlations between thermodynamics properties and equilibrium constant; able to develop mathematical equations to solve for equilibrium compositions and reaction coordinate for single and multiple reactions.	Excellent understanding on the problem, able to solve problems to determine equilibrium compositions for multiple reactions, as well as to perform analysis on the equilibrium compositions with regard to changes in the process conditions.

Appendix 2: Assessment Criteria for Class Participation

Class participation will be gauged by weekly online polls and by submitting the homework. These polls serve as a self-evaluation tool for the student, and help the faculty gauge the pulse of the class in terms of effectiveness of the learning. Points are awarded for participation and submitting the homework, regardless of whether the answers are correct/wrong.

Criteria	Grade
Polls: at least 5/6 submitted HW: All questions had a strong attempt, the HW is complete.	5% (Full points)
Polls: less than 5/6 answered HW: All questions had a strong attempt, the HW is complete.	3%
HW: One of more questions with a weak/no-attempt. The homework is considered incomplete. Such incomplete homeworks will get a 0 regardless of the number of polls addressed.	0%

Appendix 3: The EAB (Engineering Accreditation Board) Accreditation SLOs (Student Learning Outcomes)

a) **Engineering knowledge:** Apply the knowledge of mathematics, natural science, engineering fundamentals, and an engineering specialisation to the solution of complex engineering problems
b) **Problem Analysis:** Identify, formulate, research literature, and analyse complex engineering problems reaching substantiated conclusions using first principles of mathematics, natural sciences, and engineering sciences.
c) **Design/development of Solutions:** Design solutions for complex engineering problems and design system components or processes that meet the specified needs with appropriate consideration for public health and safety, cultural, societal, and environmental considerations.
d) **Investigation:** Conduct investigations of complex problems using research-based knowledge and research methods including design of experiments, analysis and interpretation of data, and synthesis of the information to provide valid conclusions.
e) **Modern Tool Usage:** Create, select, and apply appropriate techniques, resources, and modern engineering and IT tools including prediction and modelling to complex engineering activities with an understanding of the limitations
f) **The engineer and Society:** Apply reasoning informed by the contextual knowledge to assess societal, health, safety, legal, and cultural issues and the consequent responsibilities relevant to the professional engineering practice.
g) **Environment and Sustainability:** Understand the impact of the professional engineering solutions in societal and environmental contexts, and demonstrate the knowledge of, and need for the sustainable development.
h) **Ethics:** Apply ethical principles and commit to professional ethics and responsibilities and norms of the engineering practice.
i) **Individual and Team Work:** Function effectively as an individual, and as a member or leader in diverse teams and in multidisciplinary settings.
j) **Communication:** Communicate effectively on complex engineering activities with the engineering community and with society at large, such as, being able to comprehend and write effective reports and design documentation, make effective presentations, and give and receive clear instructions.
k) **Project Management and Finance:** Demonstrate knowledge and understanding of the engineering and management principles and economic decision-making, and apply these to one's own work, as a member and leader in a team, to manage projects and in multidisciplinary environments.
l) **Life-long Learning:** Recognise the need for, and have the preparation and ability to engage in independent and life-long learning in the broadest context of technological change