Faculty of Engineering and Applied Science

CHEE 311 – FLUID PHASE AND REACTION EQUILIBRIUM

Course Syllabus – Fall 2021

This is your course syllabus. Please download the file and keep it for future reference.

LAND ACKNOWLEDGEMENT

Queen's University is situated on traditional Anishinaabe and Haudenosaunee Territory.
See: http://www.queensu.ca/encyclopedia/t/traditional-territories

INCLUSIVITY STATEMENT

Queen's students, faculty, and staff come from every imaginable background – small towns and suburbs, urban high rises, Indigenous communities, and from more than 100 countries around the world. You belong here: https://www.queensu.ca/inclusive/.

TEACHING TEAM

COURSE INSTRUCTOR

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CHEE 311 (F 3-0-0.5 3.5)

Course Description[1]

This course is concerned with the application of thermodynamics to practical problems of the chemical industry. Emphasis is placed on the study of phase equilibrium, including vapour-liquid equilibrium and liquid-liquid equilibrium. Contemporary methods of calculating the thermodynamic properties of non-ideal vapours and liquids will be presented and applied. The principles of chemical reaction equilibrium will also be studied. The design component of the course will require students to perform theoretical vapour-liquid equilibrium calculations and recommend proper operating conditions for a single-stage unit (flash drum) that separates a non-ideal binary mixture.

PREREQUISITE: CHEE 210

(0/0/0/30/12)

Pre-Requisite Knowledge

This course is designed for learners with background in material and energy balances, chemical reactions, calculus, numerical methods, and basic thermodynamics.

Course Learning Outcomes (CLO)

By the end of this course, students should be able to:

CLO	Description	Indicators
CLO 1	Identify and understand the principles of chemical equilibrium thermodynamics to solve multiphase equilibria and chemical reaction equilibria.	KB-ES-Thermo (a) KB ES-Thermo (b)
CLO 2	Analyze the conditions associated with ideal and non-ideal vapour-liquid systems at equilibrium through the construction and interpretation of phase diagrams for ideal and non-ideal binary mixtures.	KB-ES-Thermo (a) KB-ES-Thermo (b)

[1] Course Author(s): KIMBERLEY B. MCAULEY, Fall 2021; Queen's University holds a license for the use of the Course Authors' Intellectual Property for CHEE 311.

CLO 3	Use empirical correlations and experimental data to evaluate thermodynamic quantities that relate to the vapour-liquid or liquid-liquid equilibria of ideal and non- ideal chemical mixtures.	KB-ES-Thermo (c)
CLO 4	Determine equilibrium constants for chemical reactions and equilibrium point compositions for multiple reaction systems.	KB-ES-Thermo (d)
CLO 5	Solve single- and multistage separation processes involving non-ideal chemical mixtures using numerical methods and simulations, and recommend appropriate operating conditions.	KB Process (c) PA-Evaluate DE-Solutions ET-Apply

COURSE EVALUATION

Deliverable	**Week or Due Date**	**Weight (%)**	**Alignment with CLOs**
Test 1, Dunning Hall 10 & 14	Sept. 27, 11:30	20	CLO1, 2
Test 2, Dunning Hall 10 & 14	Nov. 9, 11:30	20	CLO 1, 2,3
Design Project	Dec. 6, 4:30	15	CLO 5
Final Exam	Exam period	45	CLO 1, 2, 3, 4

ASSESSMENT DESCRIPTIONS

Tests

There are two tests in this course. Each test will require you to solve one or more problems and may require you to discuss your findings. More details about the tests can be found in OnQ. The tests will be open-book. You will be permitted to use the textbook, printed course slides, hand-written notes and solutions to old problems.

Design Project

The aim of this project is to perform theoretical vapour-liquid equilibrium calculations and recommend appropriate operating conditions for a flash-drum system that separates a non-ideal binary mixture. Student groups will be required to provide incremental solutions during the term. This project will be completed in groups of 3 or 4 students. Students will learn to use HYSYS software, which will be used in future CHEE courses.

Final Exam

The final exam is open book. You will be permitted to use the textbook, printed course slides, hand-written notes and solutions to old problems. Students must write their exam on the day and time scheduled by the University. You should not schedule vacations, travel, etc. during the exam period. The Term and Session Dates will indicate the final exam period session dates in each term. The final exam is open book.

GRADING

All assessments in this course will receive numerical percentage marks. The final grade you receive for the course will be derived by converting your numerical course average to a letter grade according to the established Grade Point Index.

Feedback on Assessments

The teaching team will provide feedback on graded activities. You can expect feedback on your assessments within seven days of the due date.

Assessing your Final Grade

Your final grades will show on SOLUS. Official transcripts showing final grades will be available on the Official Grade Release Date. Please note that in official transcripts, a mark of IN (incomplete) is considered a grade, and your transcript is released with this grade.

COURSE MATERIALS

Required Textbook

"*Introduction to Chemical Engineering Thermodynamics*", by Smith, Van Ness, Abbott and Swihart. The bookstore has the 9th edition, but earlier editions (with or without Swihart as a coauthor) are also fine. This textbook (referred to as "SVA" in the lecture slides) is available from the campus bookstore in hard copy and e-book formats. Extensive use of the textbook is made throughout the term, including reference to numerous tables and appendices. You will be expected to have hard-copy access to specific tables and appendices in the textbook during tests and the final exam.

Course notes and other course-related material:

All other course material is accessible via OnQ.

Required Calculator:

A Casio 991 is required. **ONLY** this type of non-programmable, non-communicating calculator will be allowed during tests and exams. Knowing how to use the Solve capability of your calculator will be helpful during tests and exam.

Course-Specific Computer-Related Skills:

This course requires computer-related technical skills. You will need to use HYSYS software for the design project. Instruction on the use of HYSYS will be provided during the Design Project tutorials shown in the Activities Schedule below.

Suggested Time Commitment:

The course duration is one semester (12 weeks plus the final exam period). Learners can expect to invest on average 7-9 hours per week in this course. Learners who adhere to a pre-determined study schedule are more likely to complete this course successfully.

Activities Schedule for CHEE 311:

Week number	Date on Monday	Monday 4:30	Tuesday 11:30-1:30	Friday 2:30
1	06-Sep		Lectures	Lecture
2	13-Sep	Design Project tutorial in cluster	Lectures	Lecture
3	20-Sep	Lecture	Lecture/Lecture	Tutorial/Q&A
4	27-Sep	Lecture	Test 1 Dunning 10 & 14	Lecture
5	04-Oct	Design Project tutorial in cluster	Lectures	Lecture
	11-Oct	Thanksgiving	Break	Break
6	18-Oct	Lecture	Lectures	Lectures
7	25-Oct	Design Project tutorial in cluster	Tutorial/Q&A	Lecture
8	01-Nov	Lecture	Lectures	Tutorial/Q&A
9	08-Nov	Lecture	Test 2 Dunning 10 & 14	Lecture
10	15-Nov	Design Project tutorial in cluster	Lectures	Lecture
11	22-Nov	Lecture	Lectures	Lecture
12	29-Nov	Design Project tutorial in cluster	Lectures	Lecture
	06-Dec	Design Project due		

Weekly Course Outcomes

Week	Learning Outcomes from Lectures	Assessment
1	**Introduction to Phase Equilibrium** By the end of this week, learners will be able to: • Describe open systems, closed systems and phases [CLO1] • Distinguish between intensive and extensive properties [CLO1] • Use phase diagrams to indentify which phases are present at a given equilibrium temperature and pressure [CLO1] • Use two-component phase diagrams to identify which phases are present and their compositions [CLO2] • Use two-component phase diagrams to perform flash calculations [CLO2]	**Test 1, Test 2 and final exam**
2	**Gibbs Free Energy and Equilibrium** By the end of this week, learners will be able to: • Describe small system changes using exact differentials • Relate Gibbs free energy and chemical potential to phase equilibrium [CLO1] • Compute volume, enthalpy, entropy and Gibb's free energy of ideal gas mixtures based on pure components [CLO1] • Compute volume, enthalpy, entropy and Gibb's free energy of ideal solutions based on pure components [CLO1] • Perform bubble point and dew point calculations using Raoult's law [CLO1]	**Test 1, Test 2 and final exam**
3	**Flash Calculations and Partition Coefficients** By the end of this week, learners will be able to: • Explain the derivation of Raoult's law [CLO1] • Explain the relationship between the lever rule and component material balances [CLO2] • Perform flash calculations using Raoult's law [CLO1] • Obtain partition coefficients from De Priester charts [CLO1] • Perform bubble point, dew point and flash calculations using partition coefficients [CLO1]	**Test 1, Test 2 and final exam**

Week	Learning Outcomes from Lectures	Assessment
4	**Equations of State and Fugacity** By the end of this week, learners will be able to: • Compute compressibility factor and molar volume of real gases using virial equation of state, Lee-Kesler correlation tables and Pitzer correlations for generalized virial equation [CLO1] • Describe the relationship between fugacity and pressure [CLO1] • Compute fugacity of real gases using generalized virial equation [CLO1] • Describe the relationship between fugacity coefficient and compressibility [CLO1] • Describe phase equilibrium condition for a single-component system using fugacity [CLO1] • Compute fugacity of a pure liquid [CLO1]	**Test 2 and final exam**
5	**Nonideal Solutions and Ideal Solutions** By the end of this week, learners will be able to: • Describe nonideal solutions in terms of excess molar volume and excess molar enthalpy [CLO1] • Express total properties in terms of partial molar properties [CLO1] • Calculate partial molar volumes from mixture molar volumes [CLO1] • Describe the relationship between fugacity of a component in a gas mixture and its partial pressure [CLO1] • Calculate fugacity coefficients in non-ideal gas mixtures using virial equation of state for gas mixtures [CLO1] • Use the Lewis-Randall rule to calculate fugacity coefficients for components in an ideal solution [CLO1] • Write phase equilibrium relationship in terms of component fugacities [CLO1] • Obtain activity coefficients from binary phase diagrams [CLO2]	**Test 2 and final exam**

Week	Learning Outcomes from Lectures	Assessment
6	**Activity Coefficients and Excess Gibbs Free Energy** By the end of this week, learners will be able to: • Compute excess Gibbs free energy using binary phase diagrams [CLO2] • Estimate parameters in Margules and Van Laar correlations using data from Pxy diagrams [CLO3] • Use Margules, Van Laar and Wilson equations to compute activity coefficients in the liquid phase [CLO3]	**Test 2 and final exam**
7	**Nonideal VLE Problems** By the end of this week, learners will be able to: • Express vapour-liquid equilibrium in terms of γ_i and Φ_i • Perform iterative bubble point and dew point calculations for nonideal multicomponent systems [CLO1][CLO3] • Make appropriate assumptions to obtain modified Raoult's law [CLO1] • Obtain partition coefficients for nonideal VLE systems and use them to perform flash calculations [CLO3]	**Test 2 and final exam**
8	**Azeotropes and Henry's Law** By the end of this week, learners will be able to: • Use relative volatilities to determine if an azeotrope exists for a binary system [CLO1][CLO3] • Determine the composition of an azeotrope [CLO3] • Describe VLE for dilute solutions using Henry's law [CLO3] • Obtain Henry's law coefficients from activity coefficient correlations [CLO1] • Perform VLE calculations using Henry's law [CLO3]	**Final exam**
9	**Liquid-Liquid Equilibrium** By the end of this week, learners will be able to: • Identify liquid-phase instability from Gibbs free energy of mixing [CLO1] [CLO3] • Perform liquid-liquid equilibrium calculations using binary and ternary phase diagrams [CLO2], [CLO3] • Perform liquid-liquid extraction calculations using ternary phase diagrams [CLO3]	**Final exam**

Week	Learning Outcomes from Lectures	Assessment
	Chemical Reaction Equilibrium	**Final exam**
10	By the end of this week, learners will be able to: • Write species mole fractions in terms of extent of reaction [CLO1][CLO4] • Express reaction equilibrium condition in terms of Gibbs free energy, chemical potential, fugacities and activities [CLO1] • Calculate equilibrium constants at 298.15 K from Gibbs free energies of formation [CLO4] • Obtain equilibrium constants at other temperatures [CLO4] • Compute equilibrium mole fractions for a gas-phase reaction [CLO4]	
11	**Chemical Reaction Equilibrium II** By the end of this week, learners will be able to: • Compute liquid-phase activities [CLO1] • Compute equilibrium composition for liquid-phase reactions [CLO4] • Perform equilibrium calculations for multiple reactions [CLO4]	**Final exam**
12	**Course Wrap-Up and Review** By the end of this week, learners will be able to: • Describe conditions for simultaneous reaction and phase equilibrium [CLO1]	**Final exam**

COURSE COMMUNICATION

NETIQUETTE

In this course, you may be expected to communicate with your peers and the teaching team through electronic communication. You are expected to use the utmost respect in your dealings with your colleagues or when participating in activities, discussions, and online communication.

Following is a list of netiquette guidelines. Please read them carefully and use them to guide your online communication in this course and beyond.

1. Make a personal commitment to learn about, understand, and support your peers.
2. Assume the best of others and expect the best of them.
3. Acknowledge the impact of oppression on the lives of other people and make sure your writing is respectful and inclusive.
4. Recognize and value the experiences, abilities, and knowledge each person brings.

5. Pay close attention to what your peers write before you respond. Think through and re-read your writings before you post or send them to others.
6. It's alright to disagree with ideas, but do not make personal attacks.
7. Be open to be challenged or confronted on your ideas and challenge others with the intent of facilitating growth. Do not demean or embarrass others.
8. Encourage others to develop and share their ideas.

QUESTIONS ABOUT COURSE MATERIAL

Questions or comments regarding the course material can asked in class, before class, or at the end of class. Questions and comments via email to the course instructor are also welcome.

COURSE ANNOUNCEMENTS

The instructor will routinely post course news in the Announcements section on the main course homepage on OnQ. Please sign up to be automatically notified by email when the instructor posts new information in the Announcements section. Instructions on how to modify your notifications are found in the **Begin Here** section of the onQ course site.

OFFICE HOURS

No scheduled office hours are planned. If you would like to meet with a TA or the instructor outside of class hours, please send an email with some suggested times and dates so we can schedule a meeting.

CONFIDENTIAL MATTERS

If you have a confidential matter you would like to discuss with Prof. McAuley, please contact her via email using the address on the first page of this document. Expect email replies within 48 hours.

STANDARD FEAS INFORMATION

COURSE POLICIES

Please review the following policies concerning copyright, academic integrity, absences and academic accommodations:

COPYRIGHT

Course materials created by the course instructor, including all slides, presentations, synchronous and asynchronous course recordings, handouts, tests, exams, and other similar course materials, are the intellectual property of the instructor. It is a departure from academic integrity to distribute, publicly post, sell or otherwise disseminate an instructor's course materials or to provide an instructor's course materials to anyone else for distribution, posting, sale or other means of dissemination, without the instructor's ***express consent***. A student who engages in such conduct may be subject to penalty for a departure from academic integrity and may also face adverse legal consequences for infringement of intellectual property rights and, with respect to recordings, potentially privacy violations of other students.

Academic Integrity

As an engineering student, you have made a decision to join us in the profession of engineering, a long-respected profession with high standards of behaviour. As future engineers, we expect you to behave with integrity at all times. Please note that Engineers have a duty to:

- Act at all times with devotion to the high ideals of personal honour and professional integrity.
- Give proper credit for engineering work

The standard of behaviour expected of professional engineers is explained in the Professional Engineers Ontario Code of Ethics. Information on policies concerning academic integrity is available in the Queen's University Code of Conduct, in the Senate Academic Integrity Policy Statement, on the Faculty of Engineering and Applied Science website, and from your instructor.

Departures from academic integrity include plagiarism, use of unauthorized materials or services, facilitation, forgery, falsification, unauthorized use of intellectual property, and collaboration, and are antithetical to the development of an academic community at Queen's. Given the seriousness of these matters, actions which contravene the regulation on academic integrity carry sanctions that can range from a warning or the loss of grades on an assignment to the failure of a course to a requirement to withdraw from the University.

In the case of online or remotely proctored exams, impersonating another student, copying from another student, making information available to another student about the exam questions or possible answers, posting materials to online services, communicating with another person during an exam or about an exam during the exam window, or accessing unauthorized materials, including internet sources and using unauthorized materials, including smart devices, are actions in contravention of academic integrity.

Late Policy

Any applicable late penalties are described in the details for each assessment. In the event of extenuating circumstances, you must follow the policies for requesting an academic consideration (please see below). Note that unacceptable reasons include extra-curricular activities, travel plans, generally behind on schoolwork, etc. In the absence of an approved consideration request, the normal late penalty will apply as described in the assignment or any course/departmental policies.

Invalid Exams

An exam may be declared invalid in case of an interruption in an in-person examination; if the instructions in a remote or online exam were not followed; if the student uploads wrong materials; or if a situation arises where the integrity of the exam cannot be verified. If an exam is declared invalid, the student may be granted a re-write.

Absences (Academic Consideration) and Academic Accommodations

For absences and academic accommodations please review the information on the FEAS website.

ACADEMIC AND STUDENT SUPPORT

Queen's has a robust set of supports available to you including the Library, Student Academic Success Services (Learning Strategies and Writing Centre), and Career Services. Learners are encouraged to visit the Faculty of Engineering and Applied Science Current Students web portal for information about various other policies such as academic advisors, registration, student exchanges, awards and scholarships, etc.

INDIVIDUAL NEEDS AND SUPPORT

If you have a disability or health-related condition that may require academic accommodations, please approach the Queen's Accessibility Services. The staff at Accessibility Services are available by appointment to develop individualized accommodation plans, provide referrals, and assist with advocacy. The sooner you let us know your needs, the better we can assist you in achieving your learning goals. For questions or assistance with requesting Academic Consideration or Accommodation, contact the FEAS Academic Accommodation Coordinator at engineering.aac@queensu.ca

Every effort has been made to provide course materials that are accessible. For further information on accessibility compliance of the educational technologies used in this course, please consult the links below.

Educational Technology	Accessibility Compliance Information
onQ (Brightspace Learning Management System by D2L)	https://www.d2l.com/accessibility/standards/
MS-Teams	https://support.microsoft.com/en-us/office/accessibility-support-for-microsoft-teams-d12ee53f-d15f-445e-be8d-f0ba2c5ee68f
Zoom	https://zoom.us/accessibility

If you find any element of this course difficult to access, please discuss with your instructor how you can obtain an accommodation.

RELIGIOUS OBSERVANCE

Students in need of accommodation for religious observance are asked to speak to their professor within a week of receiving their syllabus. Note also that alternative assignments are considered a "reasonable accommodation" under the Ontario Human Rights Code. Students with questions about their rights and responsibilities regarding religious accommodation should contact the Chaplain via Chaplain@queensu.ca.

TECHNICAL SUPPORT

Some basic comfort level with basic hardware and software skills are required for this course. If you require technical assistance, please contact Technical Support.

SUPPORTIVE PERSONAL COUNSELLING

If at any time you find yourself feeling overwhelmed, anxious, sad, lonely, or distressed, consider confidential supportive counselling offered by the embedded counselors at the Student Wellness Service Faculty of Engineering and Applied Science.