Faculty of Engineering and Applied Science

CHEE 311 – FLUID PHASE AND REACTION EQUILIBRIUM

Course Syllabus – Fall 2020

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

TEACHING TEAM

COURSE INSTRUCTOR

Kimberley B. McAuley, PhD,
P.Eng.
Chemical Engineering Queen's University

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Office hours : Mondays 8 :30-9 :30 via Zoom

TEACHING ASSISTANTS:

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Office hours: by appointment

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. (0/0/0/30/12)

PREREQUISITE: CHEE 210

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)
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)

[1] Course Author(s): KIMBERLEY B. MCAULEY, Fall 2020; Queen's University holds a licence for the use of the Course Authors' Intellectual Property for CHEE 311.

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	Sept. 28	15	CLO1, 2
Test 2	Oct. 19	15	CLO 1, 2
Test 3	Nov. 9	15	CLO 1, 2, 3
Design Project	Nov. 30	15	CLO 5
Final Exam	Exam period	40	CLO 1, 2, 3, 4

ASSESSMENT DESCRIPTIONS

Tests

There are three 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. You will not be permitted to conduct internet searches or to use other on-line materials.

Design Project

The aim of this project is to perform theoretical vapour-liquid equilibrium calculations and recommend appropriate operating conditions for a flash drum that separates a non-ideal binary mixture. Students groups will be required to provide incremental solutions during the term. This project will be completed in groups of 3 or 4 students. Information about selecting your group members is provided on the slides for the First CHEE 311 Q&A meeting. Students will learn to use HYSIS software starting on

Final Exam

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. You will be permitted to use the textbook, printed course slides, hand-written notes and solutions to old problems. You will not be permitted to conduct internet searches or to use other on-line materials.

Remote Proctoring - Proctortrack

The final exam and some tests in this course will use remote proctoring provided by a third-party, cloud-based service that enables the completion of a proctored exam or test from an off-campus location, through onQ or Elentra. This online proctoring solution was chosen as part of the approach to maintaining academic integrity in online assessment. Precise details about how remote proctoring will be used in this course can be found in the "Getting Started with Remote Proctoring" content module in onQ. When writing tests/exams using remote proctoring, you are connecting to the third-party service. Queen's has conducted a privacy and security review of the service and has entered into a binding agreement with terms that address the appropriate collection, use and disclosure of personal information in accordance with Ontario's privacy legislation. You should also take measures yourself to protect your information by keeping your NetID password and challenge questions private, closing all applications prior to starting an exam/test, and ensuring your device is updated and safeguarded against malware. For more information about remote proctoring, see the Student FAQs on the VPTL/ITS Resource page for remote proctoring.

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. The bookstore has the 8th edition, but earlier editions 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 exams.

Required Hardware/Software:

Students must have a reliable internet connection and hardware that are compatible with online learning and remote proctoring system requirements.

Course-Specific Computer-Related Skills:

This course requires computer-related technical skills. You will need to use HYSIS software for the design project. An Introduction to HYSIS Q&A session will be held on Monday, September 21 at 9:30. Further information will be posted on OnQ.

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.

Nominally, this course has 3 lecture hours + 1 tutorial hour per week with the following times reserved in the timetable: lecture and tutorial on Monday 9:30 to 11:30, lecture on Wednesday 8:30 to 9:30, and lecture Thursday on 10:30 to 11:30. As shown in the table below, some of these time slots will be used for synchronous activities. However, lectures will be delivered asynchronously, which should be beneficial for students who live in difficult time zones. Lecture slides will be supplemented with videos and real-time on-line Question-and-Answer Sessions for interactive discussions on Thursday of each week. Prior to each week's Q&A sessions, students should view the lecture slides and videos. Additional Q&A sessions may be scheduled as needed and will be announced on OnQ. TAs

will host on-line sessions on specific Mondays to provide advice on using HYSIS and completing the Design Project. The Monday slot will also be used for tests.

Prof. McAuley will hold online office hours on Wednesdays, so individual students or small groups can ask questions. To contact Prof. McAuley for help, invite her to a Zoom meeting.

Activities Schedule for CHEE 311

Date on Monday	Monday 9:30	Wednesday 8:30	Thursday 10:30
07-Sep		Intro Q&A	Q&A
14-Sep	Design Project info session	Office Hours	Q&A
21-Sep		Office Hours	Q&A
28-Sep	Test 1	Office Hours	Q&A
05-Oct	Design Project info session	Office Hours	Q&A
12-Oct	Thanksgiving	Office Hours	Q&A
19-Oct	Test 2	Office Hours	Q&A
26-Oct	Design Project info session	Office Hours	Q&A
02-Nov		Office Hours	Q&A
09-Nov	Test 3	Office Hours	Q&A
16-Nov	Design Project info session	Office Hours	Q&A
23-Nov		Office Hours	Q&A
30-Nov	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, subsequent tests 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, subsequent tests and final exam**

Week	Learning Outcomes from Lectures	Assessment
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 2, subsequent test and final exam**
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, subsequent test and final exam**

Week	Learning Outcomes from Lectures	Assessment
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 subsequent test and final exam**
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 3 and final exam**

Week	Learning Outcomes from Lectures	Assessment
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 3 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]	**Test 3 and 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 that can be of benefit to other students should be emailed to the course instructor prior to the Q&A session each Thursday. Questions may also be asked during Q&A sessions and weekly office hours.

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 class website.

OFFICE HOURS

The office hour schedule for the instructor is provided in the activities schedule above. TA office hours will be posted in the Announcements.

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.

COURSE POLICIES

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

COPYRIGHT

The material presented in this course is intended for use as part of the course at Queen's University and is the property of the instructor unless otherwise stated. Copying this material for distribution (e.g., uploading material to a commercial third-party website) can lead to a violation of Copyright law and constitutes a violation of Academic Integrity.

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 exams, impersonating another student, copying from another student, making information available to another student about the exam questions or possible answers, communicating with another person during an exam or about an exam during the exam window, or accessing 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 may request an extension to an assignment due date without penalty. Requests must be made to your instructor prior to the original due date of the assignment, and some substantiating documentation is often required (see information below on absences). Note that unacceptable reasons include extra-curricular activities, travel plans, generally behind on schoolwork, etc. In the absence of substantiating documentation, the normal late penalty will apply as described in the assignment or departmental policies.

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/
RocScience	https://www.rocscience.com/
Google Spreadsheets	https://www.google.com/accessibility/products-features/

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

ACCOMMODATIONS RELATED TO REMOTE ASSESSMENT

To have your accommodations applied to a remote-proctored exam please follow the instructions for submitting your information, as

outlined on the QSAS website. Your accommodations will be incorporated into your exam session by the Queen's University exam coordinators, on behalf of your course instructor. This information is uploaded automatically to Examity/ Proctortrack. Please note that exam accommodations that are uploaded for a specific exam are not visible to students. For example, extra time is calculated and added automatically to the exam duration but is only visible to students once they begin their exam in the Exam Portal.
If you are already registered with QSAS and you require additional accommodations related to remote-proctored exams, please consult with your QSAS advisor to update your Letter of accommodation as appropriate.

RELIGIOUS OBSERVANCE

Students in need of accommodation for religious observance are asked to speak to their professor within a week of receiving their syllabus. Please note that Rosh Hashanah falls on the eve of September 18, 2020 so students in need of accommodation should speak to their professors right away. 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 Chaplain Kate Johnson 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.

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 109 countries around the world. You belong here: https://www.queensu.ca/inclusive/