



Faculty of Engineering and Applied Science

# CHEE 222 – PROCESS DYNAMICS AND NUMERICAL METHODS

## Course Syllabus – Winter 2021

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

Queen's University is situated on traditional Anishinaabe and Haudenosaunee Territory.

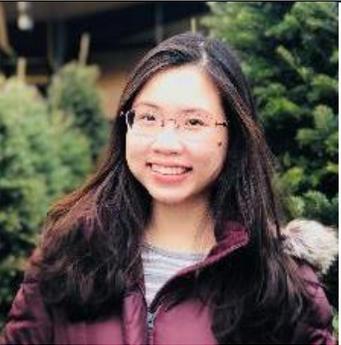
See: <http://www.queensu.ca/encyclopedia/t/traditional-territories>

## TEACHING TEAM

### COURSE INSTRUCTOR

<p><b>Kim McAuley, PhD</b> Department of Chemical Engineering Queen's University</p> <p>E-mail: <a href="mailto:kim.mcauley@queensu.ca">kim.mcauley@queensu.ca</a> Office hours: Wednesdays 8:30-9:30</p>	
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## TEACHING ASSISTANTS

<p><b>Xin (Mia) Cheng</b></p> <p>E-mail: <a href="mailto:xc11@queensu.ca">xc11@queensu.ca</a></p>	 A portrait of a young woman with long, straight brown hair, wearing a black t-shirt with a small graphic on the front. She is looking directly at the camera with a neutral expression.
<p><b>Qiujun (Abby) Liu</b></p> <p>E-mail: <a href="mailto:ql9@queensu.ca">ql9@queensu.ca</a></p>	 A portrait of a young woman with long, dark hair, wearing a dark jacket over a light-colored collared shirt. She is looking slightly to the right of the camera.
<p><b>Anh-Duong (Sunny) Vo</b></p> <p>E-mail: <a href="mailto:addv@queensu.ca">addv@queensu.ca</a></p>	 A portrait of a young woman with long, dark hair and glasses, wearing a maroon jacket. She is smiling and looking towards the camera. The background shows green foliage.

## CHEE 222 (F 3-0-0.5 3.5)

### COURSE DESCRIPTION<sup>1</sup>

Time-varying operation of chemical and biochemical processes is introduced. Dynamic mathematical models are formulated using material and energy balances. Effects of operational and design parameters on steady-state and dynamic operations are investigated. Numerical techniques are introduced to solve systems of algebraic and differential equations. Numerical and symbolic computation tools are used to analyze dynamic and steady-state process behaviour. (22/0/0/20/0)

Prerequisites: APSC 143 (Introduction to Computer Programming), CHEE 221 (Chemical Processes and Systems), MTHE 225 (MATH 225) (Ordinary Differential Equations) or permission of the department.

### PRE-REQUISITE KNOWLEDGE

This course is designed for learners with some background in computer programming, differential equations, and material and energy balances.

### COURSE LEARNING OUTCOMES (CLO)

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

CLO	DESCRIPTION	INDICATORS
CLO 1	Develop dynamic and steady-state models of chemical processes using mass balance, energy balance and constitutive relationships.	KB-Engineering Science-Process PA-Formulate
CLO 2	Calculate states, inputs or parameters at steady states via solving relevant algebraic equations.	KB-Mathematics- Numerical Methods KB-Engineering Science -Process

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<sup>1</sup> Course Author: KIM B. McAULEY. 1<sup>st</sup> Edition (initial development): WINTER 2021; Queen's University holds a licence for the use of the Course Author's Intellectual Property for CHEE 222.

CLO 3	Analyze process dynamics via solving relevant ordinary differential equations.	KB-Mathematics- Numerical Methods KB-Engineering Science - Process
CLO 4	Develop linearized models with deviation variables and solve using Laplace transforms.	KB-Mathematics- Understanding of mathematical structures KB-Engineering Science - Process
CLO 5	Solve complex algebraic and ordinary differential equations using MATLAB built-in functions, and implement classical numerical methods on MATLAB.	ET-Apply

## COURSE EVALUATION

### ASSESSMENT WEIGHTING

Assessment Tool	Due Date or Test Date	Weight	Alignment with CLOs
Test 1	Mon. Feb. 8, 8:30 a.m.	20%	1, 2
Test 2	Mon. Mar. 8, 8:30 a.m.	20%	1, 2, 3, 4
<b>Assignments</b>			
Assignment 1	Thurs. Feb. 25, 11:00 p.m.	10%	1,2,3,5
Assignment 2	Thurs. Apr. 8, 11:00 p.m.	10%	1,2,3,4,5
<b>Final Exam</b>	Final Exam Period	40%	1,2,3,4,5
		<b>100%</b>	

## ASSESSMENT DESCRIPTIONS

There are two proctored open-book tests in this course. These tests are designed to provide learners with feedback on their knowledge during the term. You will have 90 minutes to complete each test. Test dates and times are listed in the table above.

There are two assignments in this course, which will be done in groups of 2 or 3 students. In these assignments you will develop model equations describing chemical processes and solve them using Excel and MATLAB. More details about the assignments can be found in onQ.

The final exam is open-book. 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.

### Remote Proctoring - Proctortrack

The tests and final exam 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. 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 or will be provided by the instructor.

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 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 OUR Exams 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.

## Accessing 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

### Recommended Textbooks:

- Felder, R.M., Rousseau, R.W. and Bullard, L.G., Elementary Principles of Chemical Processes, 4th Edition, Wiley and Sons Inc., New York, NY (2016).
- Edwards, C.H., Penney, D.E. and Calvis, D.T., Differential Equations and Boundary Value Problems – Computing and Modeling, 5<sup>th</sup> Edition, Pearson (2014, 2019).

### 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. You will have access to Excel during your tests and final exam.

### 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. For this course, you will need to use MATLAB and Excel for the assignments. TAs will conduct online tutorials to assist students with use of MATLAB. You may also use Excel during tests and the exam.

## Suggested Time Commitment and Schedule

This course represents a study period of one semester spanning 12 weeks. 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 successfully complete the course. Lecture slides with audio will be posted in advance so that students can go through them at their own paced during the week in preparation for real-time question-and-answer sessions each Thursday, as shown in the table below. Tutorials on Mondays will focus on Matlab and Excel skills required to succeed in the assignments. Tests will be held during two of the Monday morning slots.

Professor McAuley will be available each Wednesday morning from 8:30 to 9:30. Please send her email or invite her to a Zoom or Teams meeting if you would like to schedule a discussion during these office hours.

## Synchronous Activities Schedule and Due Dates for CHEE 222

<b>Date on Monday</b>	<b>Monday 8:30</b>	<b>Wednesday 8:30</b>	<b>Thursday 8:30</b>
11-Jan	Introductory lecture via MS Teams	Office Hours	Q&A
18-Jan	Tutorial	Office Hours	Q&A
25-Jan	Tutorial	Office Hours	Q&A
1-Feb	Tutorial	Office Hours	Q&A
8-Feb	Test 1	Office Hours	Q&A
15-Feb	Family Day	Reading Week	Reading Week
22-Feb	Tutorial	Office Hours	Q&A Assignment #1 Due
1-Mar	Tutorial	Office Hours	Q&A
8-Mar	Test 2	Office Hours	Q&A
15-Mar	Tutorial	Office Hours	Q&A

22-Mar	Tutorial	Office Hours	Q&A
29-Mar	Tutorial	Office Hours	Q&A
5-Apr	Tutorial	Office Hours	Q&A Assignment #2 Due

## WEEKLY LECTURES AND OUTCOMES

Week	Learning Outcomes	Assessment
1	<p><b>Introduction to Process Modeling</b></p> <p>By the end of this week, learners will be able to:</p> <ul style="list-style-type: none"> <li>Distinguish between lumped and distributed models [CLO1]</li> <li>Develop fundamental models based on dynamic material balances [CLO1]</li> </ul>	<p><b>Tests 1 &amp; 2, Assignments, Final Exam</b></p>
2	<p><b>Steady-State and Dynamic Models</b></p> <p>By the end of this week, learners will be able to:</p> <ul style="list-style-type: none"> <li>Derive steady-state and dynamic models using material balances [CLO1]</li> <li>Assess degrees of freedom when solving systems of equations [CLO2]</li> <li>Use MATLAB and Excel to solve systems of linear equations [CLO2, CLO5]</li> </ul>	<p><b>Tests 1&amp;2, Assignments, Final Exam</b></p>

Week	Learning Outcomes	Assessment
3	<p><b>Solving Nonlinear Algebraic Equations with a Single Unknown</b></p> <p>By the end of this week, learners will be able to:</p> <ul style="list-style-type: none"> <li>Solve single equations using successive substitution, bisection, regula falsi, and Newton's method [CLO2]</li> </ul>	<p><b>Test 1, Assignments, Final Exam,</b></p>
4	<p><b>Newton's Method with Multiple Unknowns</b></p> <p>By the end of this week, learners will be able to:</p> <ul style="list-style-type: none"> <li>Explain relationship between Newton's method and Taylor series [CLO2]</li> <li>Derive nonlinear algebraic models with multiple unknowns and solve them using Newton's method [CLO1], [CLO2], [CLO5]</li> </ul>	<p>Test 2, Assignments, Final Exam</p>
5	<p><b>Solving Linear Ordinary Differential Equations</b></p> <p>By the end of this week, learners will be able to:</p> <ul style="list-style-type: none"> <li>Determine analytical solutions for linear differential equations using Laplace transforms [CLO3], [CLO4]</li> <li>Put linear differential equations into standard form to determine gain and time constants [CLO3]</li> </ul>	<p>Test 2, Assignments, Final Exam</p>
6	<p><b>More Laplace Transforms and Modeling</b></p> <p>By the end of this week, learners will be able to:</p> <ul style="list-style-type: none"> <li>Use Laplace transforms to solve multiple linear ODEs [CLO1], [CLO3], [CLO4]</li> <li>Linearize nonlinear differential equations and obtain approximate solutions [CLO4]</li> </ul>	<p>Test 2, Assignments, Final Exam</p>

Week	Learning Outcomes	Assessment
7	<p><b>Process Modeling with Energy Balances</b></p> <p>By the end of this week, learners will be able to:</p> <ul style="list-style-type: none"> <li>• Derive dynamic energy balance models [CLO1]</li> <li>• Express models with multiple ODEs using vector notation [CLO3]</li> </ul>	Assignments, Final Exam
8	<p><b>Numerical Methods for Ordinary Differential Equations</b></p> <p>By the end of this week, learners will be able to:</p> <ul style="list-style-type: none"> <li>• Use explicit and implicit Euler’s method to solve ODE initial value problems [CLO3], [CLO5]</li> <li>• Distinguish between initial value problems and boundary value problems [CLO3]</li> </ul>	Assignment 2, Final Exam
9	<p><b>Numerical Methods for Ordinary Differential Equations (2)</b></p> <p>By the end of this week, learners will be able to:</p> <ul style="list-style-type: none"> <li>• Use 2<sup>nd</sup> order and 4<sup>th</sup> order Runge-Kutta methods to solve individual ODEs and systems of ODEs [CLO3], [CLO4]</li> <li>• Use Runge-Kutta-based MATLAB routines to solve systems of ODEs [CLO5]</li> </ul>	Assignment 2, Final Exam
	<b>Numerical Integration and Cubic Splines</b>	Final Exam
10	<p>By the end of this week, learners will be able to:</p> <ul style="list-style-type: none"> <li>• Perform numerical integration using trapezoidal rule and Simpson’s rule [CLO2], [CLO5]</li> <li>• Fit cubic splines through data points [CLO2], [CLO5]</li> </ul>	

Week	Learning Outcomes	Assessment
11	<b>Advanced Differential Equations for Chemical Processes</b>	Final Exam
	By the end of this week, learners will be able to:	
	<ul style="list-style-type: none"> <li>Derive and solve steady-state ODEs involving one spatial variable [CLO1], [CLO5]</li> <li>Derive second-order differential equations and partial differential equations based on material and energy balances [CLO1]</li> </ul>	
12	<b>Course Wrap-Up</b>	Final Exam
	By the end of this week, learners will be able to:	
	<ul style="list-style-type: none"> <li>Summarize modeling techniques and numerical methods covered in the course [CLO1], [CLO4]</li> <li>Derive and solve model equations in preparation for final exam [CLO1], [CLO2], [CLO3], [CLO4], [CLO5]</li> </ul>	

## 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 be asked during office hours or during the weekly Q&A sessions. Please feel free to also send questions via email to the instructor prior to the Q&A sessions.

## **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**

In addition to interaction in the Q&A discussion forums, you will have the opportunity to interact in a synchronous fashion with either a TA or the instructor. The instructor will be available during office hours at 8:30 on Wednesdays. Meetings with a TA can be requested by sending email to the TA.

## **CONFIDENTIAL MATTERS**

If you have a confidential matter you would like to discuss with your instructor, her contact details are 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

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 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 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.

## **ABSENCES (ACADEMIC CONSIDERATIONS) AND ACADEMIC ACCOMMODATIONS**

For absences and academic accommodations please review the information on the [FEAS website](#).

## **RECORDING SYNCHRONOUS (LIVE) CLASSES**

Except for the opening lecture, all lectures will be delivered asynchronously. Question-and-answer sessions and tutorials will be delivered live through a video conferencing platform supported by the University [MS Teams]. Steps have been taken by the University to configure this platform in a secure manner, and to maintain student privacy while delivering courses remotely. Please note the following:

- Attendance and question-and-answer sessions and tutorials is recommended. Some of these sessions may be recorded so that students may view them at an alternative time.

To learn more about how your personal information is collected, used and disclosed by Queen's University, please see the general [Notice of Collection, Use and Disclosure of Personal Information](#).

## **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](mailto: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.

<b>EDUCATIONAL TECHNOLOGY</b>	<b>ACCESSIBILITY COMPLIANCE INFORMATION</b>
onQ	<a href="https://www.d2l.com/accessibility/standards/">https://www.d2l.com/accessibility/standards/</a>
MS-Teams	<a href="https://support.microsoft.com/en-us/office/accessibility-support-for-microsoft-teams-d12ee53f-d15f-445e-be8d-f0ba2c5ee68f">https://support.microsoft.com/en-us/office/accessibility-support-for-microsoft-teams-d12ee53f-d15f-445e-be8d-f0ba2c5ee68f</a>

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 [Proctortrack / Examity](#).

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. 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](mailto: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/>.