Chemical Engineering 2E04: Covid-19 Edition

Numerical Methods and Computing for Chemical Engineers

Course Outline - Fall 2020

Course Details

Instructor:		**Dr. Jake Nease**	**che2e4instructor@gmail.com** **(905) 599-3165**	**BSB/B105**
Teaching Assistants:		Abhishek Premachandra	premacam@mcmaster.ca	MS Teams
		Wajdi Alnoush	alnoushw@mcmaster.ca	MS Teams
		Blake Patterson	pattebe@mcmaster.ca	MS Teams
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Website:		Avenue2Learn	avenue.mcmaster.ca	
Lectures:		Tu/We/Fr	12:30 – 13:20	MS Teams
Tutorials/Labs:	T01	Monday	10:30 – 12:20	MS Teams
	T02	Wednesday	10:30 – 12:20	MS Teams
	T03	Tuesday	10:30 – 12:20	MS Teams
	T04	Friday	14:30 – 16:20	MS Teams

Extra `MATLAB` *help sessions may be scheduled by TAs*

Office Hours: Wednesdays 13:30 – 16:20, or by **drop in** via video call. **Always** happy to help.

Prerequisites: Registration in Chemical Engineering or Materials Engineering, MATH 1ZA3/B3/C3

Software: `MATLAB`

Course Materials: Lecture modules, tutorials, challenges, videos, and solutions will be posted on A2L
Grades will also be posted on A2L but are not official until released on MOSAIC

Recommended Textbook: A. Gilat, V. Subramaniam: *Numerical Methods for Engineers and Scientists.* Wiley. Third Edition (2014): Wiley E-Book Campus Book Store

Formal Course Description

Chemical Engineering 2E04 focuses on the formulation and solution of various engineering problems. We review a variety of techniques for numerical solution of linear and nonlinear model equations, including algebraic and ordinary differential equations, and the use of curve-fitting and interpolation methods.

Informal Course Description

A course dedicated to solving **very hard problems** by approximating them as a ***bunch of easier problems*** solved efficiently and with high precision to minimize the errors introduced via simplification.

Learning Objectives

After completing this course, the student should be able to:

- Recognize when numerical methods should be applied as a part of a solution to a variety of chemical engineering (and other) problems or opportunities.
- Formulate mathematical models of common engineering unit operations and processes.
- Identify the appropriate algorithm or numerical method suitable for the solution.
- Break down how an algorithm works based on fundamental mathematical concepts.
- Implement algorithms using calculators and (more importantly) software tools.
- Derive algorithms for new problems based on a fundamental understanding of the objective.
- Use a numerical solution to help solve the original problem of interest.
- Identify the critical differences, advantages, and disadvantages of numerical versus analytical techniques.

Evidence of Objectives

Evidence to prove that one has achieved the above objectives may be demonstrated by:

- Explaining to a peer the fundamental concepts which are used in an algorithm.
- Using graphs and tables to illustrate how an algorithm works.
- Deriving potential algorithms to solve a problem from fundamental concepts.
- Coding an algorithm in a software tool such as `MATLAB` and proving that it works.
- Executing part of an algorithm "by hand" to show an understanding of core applied mathematics.
- Suggesting alternative algorithms for previously unsolved problems.
- Implementing the results of an algorithm in the final solution of the original problem.
- Explaining the importance of solving a problem (with or without numerical methods) in the first place.

Grading Policies

Please be aware of the following grading policies for ChE 2E04:

- Late submissions of any take-home portions of exams will not be accepted without an appropriate MSAF.
- Valid MSAF submissions will result in either a make-up examination or rolling of that component's weight into the final exam, depending on the situation.
- All assessments in this course are open-book (any book) and open-notes (any hard copies).
- Any calculator, but not computers, may be used for in-person examinations.
- The instructor retains the right to modify course weights or components; this is typically only enforced for the student's benefit. All grades are **unofficial** until final grades are posted on MOSAIC.
- Final grades will be converted to the standard McMaster 12-point scale.
- All submissions for challenges, projects, and take-home examinations must be done **electronically**.
- Any copying of code, formulations, or interpretations from other students, prior versions of this course, or resources online will be considered a violation of McMaster's academic integrity policy.
- **C19 ADJUSTMENT –** There will be no in-person exams for the 2020 offering of 2E04. See grading breakdown.

Grading Breakdown

Weight	Component	Comments
0%	Tutorial Activities	Are there for your benefit and practice. Do them in groups!
75%	Challenges	Basically the entire course's assessment. Groups of ≤ 3 students. One must be done individually. Worth 10/10/12.5/12.5/15/15% from {worst result} → {best result}.
0%	Midterm Tests	There will be no tests in ChE 2E04 this year.
20%	Take-Home Exam	Individual challenge. Administered over three days in December.
5%	Participation	Attendance in tutorial sessions (0.5% each, up to 10 sessions)

NEW FOR C19 – 2E04 Portfolio Challenges

This is a new format for assessment in this course for this year. In past years, assignments were optional but there were numerous midterms and a coding examination. Due to the **C19** pandemic, I have decided to forego formal examinations and instead focus on letting you, the students, work on some open-ended **challenges**. These challenges will test your understanding and application of course concepts and will be worth a substantial portion of your final grade. Please note the following **important** procedures:

- Challenges may be completed in groups of **up to three (3) students**.
    - All challenges can be done individually if desired.
    - AT LEAST **ONE (1)** challenge **must** be completed individually.
    - You may attack each challenge with a different group if you wish.
- Each challenge will be **worth an average of 12.5%** of your final grade.
    - Your best two results will each count for 15%.
    - Your worst two results will each count for 10%.
    - Completing the challenge individually or in groups has no impact on this distribution.
    - The instructor reserves the right to re-distribute weight **in your favour** depending on how this assessment scheme goes (this is a new idea, so we will see!).
- Challenges must be submitted **electronically** via the A2L drop box prior to the due date.
    - **Only one** group member should submit the challenge.
    - Your submission must be **typeset** using a word processor and will be held to a high standard of technical writing and formatting. You may lose points for especially sloppy work.
    - Your submission report must include all **answers and plots** for the challenge, and all `MATLAB` code must be submitted as a .zip file with your report.
- MSAFs will result in an **extension** for any challenge or deferral to the take-home exam in extreme cases.

NEW FOR C19 – Take-Home Examination

Due to the nature of the pandemic and to lower examination burden/stress, there will be no formal written final exam for ChE 2E04 in 2020. Instead, you will be given a take-home problem that is shorter than a typical challenge assessment but must be completed in limited time.

- The take-home examination is **mandatory** and can be completed in **groups of up to two (2)**.
- The take-home examination will be distributed during the exam break at an optimal time for all. No MSAFs will be permitted for this examination.

Academic Honesty

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. The online nature of courses during the **C19 pandemic** will test these principles like never before.

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. **Note that these consequences will be enforced even when submitting OPTIONAL components**. 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.

- All marked **challenges are to be done individually or in your group only**, with no additional collaboration. I will facilitate discussion boards to allow you to help each other out.
- Tutorials will not be marked. Feel free to work in groups or get outside help. They are for your understanding and skill development. If you work better alone, do it alone.
- Plagiarism, improper collaboration, copying unauthorized tests or aids, and other academic dishonesty will not be tolerated. **Your first offence will be reported** to the Office of Academic Integrity.
- The default penalty for academic dishonesty is a zero on the entire challenge / assignment / exam, even if the dishonesty occurred on just one portion or question of that challenge/ assignment / exam. However, if Academic Integrity chooses to hold a hearing, they will determine the penalty.

Accessibility and Mental Health

The instructor aims to make this class accessible to all students. Please forward and optionally discuss any accommodation granted by Student Accessibility Services (SAS) with the instructor *before the third week of the course*. Please raise any other accessibility issues with the instructor as soon as possible, e.g. accessibility of the course website and course materials.

I am certified with the McMaster Professor Hippo on Campus Program for mental health awareness and aid to students in need. My office (or online video portal) is a **safe space** to discuss issues both academic and otherwise, and you are welcome to contact me at any time to chat. If I reach out to you at any time, be aware that it is not to embarrass or penalize you; it is because I care.

Course Feedback

Please do not hesitate to let me know your thoughts on the course or what you might want to change at any time. You can reach me at neasej@mcmaster.ca or che2e4instructor@gmail.com. If you would prefer to leave feedback **anonymously**, do not hesitate to use our anonymous 2E04 course feedback form.

Class Recordings – C19 Edition

I am keenly aware that coming to class live is not always possible. Although I strongly recommend that you attend lectures and tutorials live, if you must miss for any reason please note that all live lectures will be recorded.

NEW FOR C19 this year I will also be recording 5-minute post-lecture "lightning reviews" of the topics covered in that class. This will act as a quick reference for those that missed lecture or would like a recap of the most important concepts covered that day. Workshop activities will not be completed in these videos.

Class Coding Sessions

Quite frequently in this course we will be using our engineering knowledge and material covered in lecture to derive algorithms to achieve a variety of outcomes. Frequently, especially toward the beginning of the course, we will then code these algorithms together in class to see their implementation in real-time. Some of the codes will use pre-built functions or even previous codes we have developed! Challenges may also refer to these codes. All codes will be posted on A2L for you to use freely with permission.

Tutorials

Note that although tutorials are not graded, it is strongly recommended that students work through them at their own pace. Each tutorial (and challenge) contains important information relevant to the course and is fair game for assessment. Tutorial time may also be used to work on **challenges**, but the instructional team's time will be prioritized to helping students with the tutorial activities.

C19 ADJUSTMENT – All tutorials will be facilitated using breakout channels on MS Teams. You may therefore come to **any tutorial section that fits your schedule** even if you come to more than one per week. You will not receive extra credit for attending additional tutorials.

C19 ADJUSTMENT – During tutorial time, you may be "present" in the main tutorial channel on MS teams to ask questions as you work through your activity. **However**, I strongly suggest you connect with some peers in a smaller breakout channel and tackle the activity as a team. The TAs and I will bounce around between breakout channels to offer our help and check in on your progress. Your attendance will be tracked through a sign-in form that will be available during tutorial time.

Anticipated Tutorial Breakdown

Tutorial Number	Week Starting…	Expected Topic (Subject to change)
Tutorial 0	September 07	Introductions, practice activities, icebreakers (We/Fr ONLY)
Tutorial 1	September 14	Solving basic problems with MATLAB
Tutorial 2	September 21	Creating and using functions
Tutorial 3	September 28	Modeling and advanced linear systems
Tutorial 4	October 05	LU decomposition
N/A	*Reading Week*	*Suggestion: The Moon is a Harsh Mistress (Heinlein)*
Tutorial 5	October 19	Basic nonlinear systems
Tutorial 6	October 26	Advanced nonlinear systems
Tutorial 7	November 02	Polynomial model regression
Tutorial 8	November 09	Spline interpolation
Tutorial 9	November 16	Numerical differentiation
Tutorial 10	November 23	Numerical integration
Tutorial 11	November 30	ODE integration of chemical systems

** Note that tutorial topics and timing are subject to change.*

Assumed Knowledge and Getting Help

MATLAB is one of the key tools which you will learn to use in this course. MATLAB is both a programming language and a math tool. All chemical engineering students are required to complete both a programming course in their first year and use MATLAB in their second-year math courses. This course will aim to equip students to use MATLAB in the future and be more successful in their math courses.

This course is built assuming that students are at least familiar with concepts covered in first year, such as:

- Basic program flow
- Variables and memory
- IF statements
- FOR loops and WHILE loops
- Functions
- Basic data plotting

To help students, a variety of learning aids have been posted on the course website:

Recitations: Teaching assistants will lead optional weekly review sessions called Recitations where time will be devoted to the review of lecture or challenge material.

Videos: ChE 2E04 has a YOUTUBE channel!
Numerical Methods ChE McMaster

- Ep 1: Intro and Basics
- Ep 2: Matrices and Matrix Math
- Ep 3: For Loops and Pretty Graphs
- Ep 4: Functions! Functions! Functions!
- Ep 5: While loops, If Statements, & Breakpoints

Skills Test: A multiple choice self-test which you can use to identify areas for improvement, along with links to online videos or textbook sections to find the missing information. It is the result of years of experience and was originally written by Dr. Adams, who has let us use them for our iteration of this course (see what I did there?). *The skills test will be released after the first few weeks of lecture and tutorial for you to self-assess your progress!*

Computation Guides: Supplementary information to help better understand concepts in programming and numerical methods. Again, these have been generously provided by Dr. Adams from his years of experience with 2E04. These guides can be found on the course website as well.

Guide 1: Computational Complexity

Guide 2: Thinking like a Computer

Guide 3: Variable Scope

Other McMaster MATLAB Guides:

Guide 1: MATLAB Primer written by a former McMaster prof

Guide 2: MATLAB Presentation written by former graduate students

Guide 3: Making Friends with MATLAB (Module 0) developed by our own 2E04 student team

Anticipated Course Schedule and Topics (SUBJECT TO CHANGE)

Below is an outline of the topics I hope to cover in this course. This schedule is subject to change, especially in the early-goings as we get our bearings around MATLAB. *Topics in italics are only going to be covered if the pace of the class permits*. Note that each module is expected to take (roughly) 1-2 weeks, depending on size.

Module	Primary Module Topics	Content (subject to change)
Module 01A	Course Overview Linear Systems of Equations	• Overview of course structure • Linear system modeling • Language and lingo • Expansion to discretized systems
Module 01B	Linear System Solutions: Elimination Methods	• Gauss elimination • Gauss-Jordan elimination • LU decomposition • Trade-Offs and applications • Pivoting
Module 01C	Linear System Solutions: Iterative Methods	• Jacobi method • Gauss-Seidel method • Diagonal dominance • Smoothing • Condition numbers
Module 02A	Nonlinear Systems: Formulation and Bracketing	• Formulating nonlinear problems • Bisection for univariate solutions • Regula-Falsi for univariate equations • Rates of convergence
Module 02B	Nonlinear Systems: Open Methods and Multivariate Solutions	• Secant method • Review: Taylor Series expansion • Newton-Raphson method • Multivariate Newton-Raphson method
Module 03A	Curve Fitting: Regression	• Concept of regression and optimization • Linear regression • Polynomial regression • Basis function regression
Module 03B	Curve Fitting: Interpolation	• *Lagrange polynomials* • *Splines* • Data scaling and normalization
Module 04A	Numerical Differentiation	• Finite differences • Partial derivatives • *Derivatives via curve fitting* • Error analysis
Module 04B	Numerical Integration	• Newton-Cotes formulas and error analysis • Richardson extrapolation • *Romberg integration* • *Multiple integrals*
Module 05A	Univariate Differential Equations	• Defining ODEs • Methods of solving ODEs
Module 05B	Multivariate Differential Equations	• *Multivariate Euler's, and RK4 methods*

C.E.A.B. Graduate Attributes

Certain courses in the chemical engineering curriculum collect indicator data related to the development of the attributes deemed critical for engineers according to the Canadian Engineering Accreditation Board (CEAB). These indicators will be assessed throughout the course and redacted samples of student work may be collected for submission to the CEAB during McMaster Engineering's accreditation cycle. The indicators assessed in ChE 2E04 are as follows:

1.3 – Competence in engineering fundamentals.
5.2 – The ability to use modern state-of-the-art tools.
5.3 – The ability to create, adapt, modify and extend tools and techniques to solve problems.

The P.R.O.C.E.S.S.

As some of you may already be aware, the department of Chemical Engineering has a storied history of education. In addition to teaching and learning, the department is proud of our graduates not only for their academic success, but their more intrinsic traits that make them respected members of the engineering community.

Recently, several high-ranking graduates from the McMaster Chemical Engineering Program employed in various industries (oil/gas, financials, *etc*.) were interviewed to ask what traits they look for when hiring for engineering positions. Using this information, the department would like to present to you the **PROCESS**: a code of conduct that we hope will guide our students throughout this program and their careers to come.

- **P**rofessionalism
- **R**esponsibility
- **O**wnership
- **C**uriosity
- **E**mpathy
- **S**elflessness
- **S**ervice

It is up to YOU to interpret these traits and apply them to your time at McMaster and your career as you see fit. These traits will not be assessed for grades but will be strongly encouraged throughout your time at McMaster. We hope that you identify with these character traits and what they mean to you, and that you **trust the process**.

~The following two pages are required by the university senate for the 2020 fall term~

COURSE OUTLINE – APPROVED ADVISORY 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. **It is your responsibility to understand what constitutes academic dishonesty.**

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. For information on the various types of academic dishonesty please refer to the *Academic Integrity Policy*, located at https://secretariat.mcmaster.ca/university-policies-procedures-guidelines/

The following illustrates only three forms of academic dishonesty:

- plagiarism, e.g. the submission of work that is not one's own or for which other credit has been obtained.
- improper collaboration in group work.
- copying or using unauthorized aids in tests and examinations.

AUTHENTICITY / PLAGIARISM DETECTION

Some courses may use a web-based service (Turnitin.com) to reveal authenticity and ownership of student submitted work. For courses using such software, students will be expected to submit their work electronically either directly to Turnitin.com or via an online learning platform (e.g. A2L, etc.) using plagiarism detection (a service supported by Turnitin.com) so it can be checked for academic dishonesty.

Students who do not wish their work to be submitted through the plagiarism detection software must inform the Instructor before the assignment is due. No penalty will be assigned to a student who does not submit work to the plagiarism detection software. **All submitted work is subject to normal verification that standards of academic integrity have been upheld** (e.g., on-line search, other software, etc.). For more details about McMaster's use of Turnitin.com please go to www.mcmaster.ca/academicintegrity.

COURSES WITH AN ON-LINE ELEMENT

Some courses may use on-line elements (e.g. e-mail, Avenue to Learn (A2L), LearnLink, web pages, capa, Moodle, ThinkingCap, etc.). Students should be aware that, when they access the electronic components of a course using these elements, 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 a course that uses on-line elements will be deemed consent to this disclosure. If you have any questions or concerns about such disclosure please discuss this with the course instructor.

ONLINE PROCTORING

Some courses may use online proctoring software for tests and exams. This software may require students to turn on their video camera, present identification, monitor and record their computer activities, and/or lock/restrict their browser or other applications/software during tests or exams. This software may be required to be installed before the test/exam begins.

CONDUCT EXPECTATIONS

As a McMaster student, you have the right to experience, and the responsibility to demonstrate, respectful and dignified interactions within all of our living, learning and working communities. These expectations are described in the *Code of Student Rights & Responsibilities* (the "Code"). All students share the responsibility of maintaining a positive environment for the academic and personal growth of all McMaster community members, **whether in person or online**.

It is essential that students be mindful of their interactions online, as the Code remains in effect in virtual learning environments. The Code applies to any interactions that adversely affect, disrupt, or interfere with reasonable participation in University activities. Student disruptions or behaviours that interfere with university functions on online platforms (e.g. use of Avenue 2 Learn, WebEx or Zoom for delivery), will be taken very seriously and will be investigated. Outcomes may include restriction or removal of the involved students' access to these platforms.

ACADEMIC ACCOMMODATION OF STUDENTS WITH DISABILITIES

Students with disabilities who require academic accommodation must contact Student Accessibility Services (SAS) at 905-525-9140 ext. 28652 or sas@mcmaster.ca to make arrangements with a Program Coordinator. For further information, consult McMaster University's *Academic Accommodation of Students with Disabilities* policy.

REQUESTS FOR RELIEF FOR MISSED ACADEMIC TERM WORK

McMaster Student Absence Form (MSAF): In the event of an absence for medical or other reasons, students should review and follow the Academic Regulation in the Undergraduate Calendar "Requests for Relief for Missed Academic Term Work".

ACADEMIC ACCOMMODATION FOR RELIGIOUS, INDIGENOUS OR SPIRITUAL OBSERVANCES (RISO)

Students requiring academic accommodation based on religious, indigenous or spiritual observances should follow the procedures set out in the RISO policy. Students should submit their request to their Faculty Office ***normally within 10 working days*** of the beginning of term in which they anticipate a need for accommodation or to the Registrar's Office prior to their examinations. Students should also contact their instructors as soon as possible to make alternative arrangements for classes, assignments, and tests.

COPYRIGHT AND RECORDING

Students are advised that lectures, demonstrations, performances, and any other course material provided by an instructor include copyright protected works. The Copyright Act and copyright law protect every original literary, dramatic, musical and artistic work, **including lectures** by University instructors

The recording of lectures, tutorials, or other methods of instruction may occur during a course. Recording may be done by either the instructor for the purpose of authorized distribution, or by a student for the purpose of personal study. Students should be aware that their voice and/or image may be recorded by others during the class. Please speak with the instructor if this is a concern for you.

EXTREME CIRCUMSTANCES

The University reserves the right to change the dates and deadlines for any or all courses in extreme circumstances (e.g., severe weather, labour disruptions, etc.). Changes will be communicated through regular McMaster communication channels, such as McMaster Daily News, A2L and/or McMaster email.