McMaster University | SCIENCE
Department of Chemistry & Chemical Biology

We recognize and acknowledge that McMaster University meets and learns on the traditional territories of the Mississauga and Haudenosaunee nations, and within the lands protected by the "Dish With One Spoon" wampum, an agreement amongst all allied Nations to peaceably share and care for the resources around the Great Lakes.

CHEM 3PC3 - Mathematical Tools for Chemical Problems

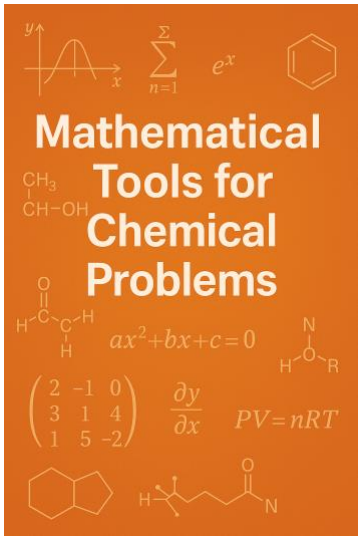
2025 FALL Term

Instructor: Rodrigo A. Vargas-Hernández| **E-mail:** vargashr@mcmater.ca | **Office: ABB 266**

Instructional Assistant: Alexandre de Camargo | **E-mail:** decamara@mcmaster.ca

Section	C01
Instructor	Rodrigo A. Vargas-Hernández
Contact Info	vargashr@mcmater.ca decamara@mcmaster.ca
Class Schedule	Thursday 8:30AM - 10:20AM Tuesday 9:30AM - 10:20AM
Location	ETB 227
Office Hours	Tuesdays 3:30 PM
Location	ABB 266
Tutorial Schedule	Tuesday 1:30 PM – 2:20 PM
Location	HH 102

Course Description



This course covers essential mathematical topics as tools for solving problems in chemistry. The theme of the first part of the course is thermodynamics calculations. The second part is concerned with linear algebra. Chemical problems associated with equilibrium and kinetics are introduced and solved via calculus and linear algebra. As such, linear algebra - solving systems of linear equations, matrix algebra, eigenvalues and eigenvectors – and some multivariate calculus topics are introduced in a physical context. The course will also cover a brief introduction to model regression algorithms like neural networks.

- One of the main focuses of the course is the development of coding skills, specifically Python.
- Instruction on the associated programming skills will be provided in tutorials.

Course and Learning Objectives

At the end of the course, the student will have elementary algebra, calculus, and programming skills tailored to model chemical systems.

Materials & Fees

Required Materials

You will need your personal computers to for the in-class coding exercises.

Resources

This course does not follow a specific book as it designed to be a collection of topics that are relevant for a common undergraduate program in chemistry. However, if the student wants to consult here are some recommended books:

1. AMPC: Applied mathematics for Physical Chemistry, James R. Barrante.
2. MPC: Mathematics for Physical Chemistry, Donald A. McQuarrie.
3. PC: Physical Chemistry, Ira N. Levine.
4. LAWA: Linear Algebra with applications, Gareth Williams.
5. MQM: Mathematics for Quantum Chemistry, Jay Martin Anderson.
6. NMSE: Numerical Methods for Scientists and Engineers, R. W. Hamming.

Notes from previous years wrote by profs. Randy Dumont and Paul Ayers will also be shared.
All content will be posted on Avenue.

Course Overview and Assessment

Week	Dates	Topic	Book	Chapter
1	Sept. 2-4	Univariate Calculus and Series: Thermodynamic, heat capacity and integration	PC	1
2	Sept. 9-11		MPC	1,2
3	Sept. 16-18	Multivariate Calculus: Fundamental Equations of Thermodynamics	PC	2,3
4	Sept. 23-25		AMPC MPC	4,7 12
5	Sept. 30 – Oct. 2	Linear Algebra: Simple and complex equilibrium	LAWA	1
6	Oct. 7-9		PC	4
7	Oct. 13-19	**Fall break. No classes this week!!**		None
	TBD	Midterm exam		
8	Oct. 21-23	More Linear Algebra: Equilibrium and steady state solutions	LAWA	2,3
9	Oct. 28-30		PC	9
10	Nov. 4-6	Orbitals and decay to equilibrium: Eigenvalues and eigenvectors	MPC	16
11	Nov. 11-13		MPC	19

12	Nov. 18-20	Regression and classification: 1. Linear regression 2. Neural Networks 3. Classification	LAWA	7
13	Nov. 25-27		NMSE	7
14	Dec. 2-4		Class notes	None
	TBD	Final exam		

Evaluation

Assessment Method	Weight
Weekly Quizzes*	20%
2 Python assignments (dates TBD)	20%
Mid-Term Exam	25%
Final Exam	35%
Total	100%

Modifications to this evaluation scheme may happen during the term but will be communicated to the class.

***Weekly Quizzes**: The deadline for each quiz is next week tutorial (Tuesdays 2:30 PM).

There are three types of quizzes, each with its own submission method. Please follow these instructions carefully to ensure your work is accepted.

1. **Coding Quizzes:**
   These must be submitted electronically by email to decamara@mcmaster.ca.
   Important: You must use the following naming template for your submission file:
   STUDENT_SURNAME_STUDENT_ID_QUIZ_NUMBER.ipynb
   (e.g., SMITH_001234567_QUIZ_2.ipynb).
2. **Exercises with Mathematical Calculations (Pencil and Paper):**
   These must be submitted in person to the teaching assistant (monitor) by the end of the tutorial section in which they are due.
   Alternative submission: If you cannot submit in person, you may leave your work in the mailbox located in the main office, specifically in the Dr. Vargas-Hernandez folder. Ensure your name, student ID, and tutorial number are clearly written on the submission.
3. **Combined Math and Coding Exercises:**
   For these exercises, you must complete both parts:
   - Coding Part: Email your code to decamara@mcmaster.ca, using the required file naming template: STUDENT_SURNAME_STUDENT_ID_QUIZ_NUMBER.ipynb.
   - Math Calculations Part: Submit your pencil and paper calculations in person during the tutorial session in which they are due. Alternatively, they may be left in the Dr. Vargas-Hernandez folder in the main office mailbox.

   Both parts must be submitted by the deadline for your work to be considered complete.

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 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.

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.*

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.

Academic Integrity in the era of Generative AI

As a researcher in the field of machine learning and AI, I recognize the significant potential of these modern tools to enhance the learning process. I support their responsible use, with the understanding that the author who submits the work is ultimately accountable for its content and any potential repercussions. In this course, where the primary objective is to develop students' mathematical and coding skills, it is essential to ensure that all work reflects genuine analysis and understanding.

The instructor and TA will be vigilant in identifying any instances of "copy-paste" answers, particularly those that appear to be generated by AI without sufficient student comprehension. If the instructor or TA suspects that an answer has been directly copied from a chatbot, the student will be required to explain their reasoning. Responses such as **"this is what ChatGPT told me"** will not be tolerated. Based on the explanation provided, appropriate consequences may be determined.

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 the McMaster Office of Academic Integrity's webpage.

Conduct Expectations

As a McMaster student, you have the right to experience, and the responsibility to demonstrate, respectful and dignified interactions within all 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.

Copyright, Recording & Research Ethics

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 only by the instructor for the purpose of improvement. 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.