# Chemical Engineering 4G03

*Optimization Formulation and Solution*

Course Outline - Winter 2020

## Course Details

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|---|---|---|---|---|
| **Instructor:** | | **Dr. Jake Nease** | **che4g3instructor@gmail.com**<br>**+1 (905) 599-3165** | **BSB/B105** |
| **Teaching Assistants:** | | Emma Hermonat<br>Mahir Jalanko<br>Alireza Shamsabadi | hermonek@mcmaster.ca<br>jalankmd@mcmaster.ca<br>shahinsa@mcmaster.ca | JHE/370<br>JHE/370<br>ETB/301 |
| **Website:** | | Avenue2Learn | avenue.mcmaster.ca | |
| **Lectures:** | | Thursday | 09:30 – 11:20 | JHE/326H |
| **Tutorials:** | T01<br>T02 | Monday<br>Wednesday | 14:30-16:20<br>12:30-14:20 | BSB/249<br>BSB/249 |
| | | *Tutorials begin January 13*<br>*Tutorials are MANDATORY and will be used to introduce software, work on practice activities, give project consultation time, and cover lecture material* | | |
| **Office Hours:** | **JAKE**:<br>**TAs**: | Mondays/Wednesdays 08:30-09:30, or by appointment (always happy to chat)<br>By appointment | | |
| **Prerequisites:** | ChE {2O04, 3E04, 3P04, 3G04, 3M04} | | | |
| **Software:** | MATLAB – Expected prerequisite but will be refreshed throughout the term<br>EXCEL – Expected prerequisite but will be refreshed throughout the term<br>GAMS – **G**eneral **A**lgebraic **M**odel **S**olver (will be introduced in this course) | | | |
| **Course Materials:** | Lecture modules, tutorials, assignments, readings, and solutions will be posted on A2L<br>Grades will also be posted on A2L but are not official | | | |
| **Recommended Textbook:** | R. Rardin: *Optimization in Operations Research*. Pearson Education | | | |
| | First Edition (1997): | | Pearson | Amazon |
| | Second Edition (2017): | | Pearson | Amazon |

## Formal Course Description

Chemical Engineering 4G03 focuses on the application of optimization methods to important engineering problems in thermodynamics, statistics, design, control, economics and scheduling. The course will emphasize problem definition, model formulation and solution analysis, with applications of existing algorithms and software tools to solve industry-related problems.

## Informal Course Description

A course dedicated to determining the **best way** to do something given a **clear objective** and set of **constraints**.

## Learning Objectives

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

- Demonstrate the concept of identifying the **best outcome** possible for a given problem
- Recognize and exploit opportunities for optimization in **real-world scenarios**
- Compare the trade-offs between **accuracy** and **computational effort**
- Demonstrate that mathematical models have **inherent errors** that can be minimized through appropriate **solution methods**, sensitivity **analysis tools** and **interpretation** of results
- Apply problem-solving strategies that can **translate a real-world problem** or opportunity into a **mathematical model** to be solve via optimization
- Interpret and explore the mathematical concepts that define the basis for **optimization theory**
- Test, debug, and apply mathematical strategies for optimization using a variety of **software tools**
- **Explain** an optimal solution and other results to an **audience that is unfamiliar** with formal optimization
- Select appropriate **model complexity** to achieve the **desired accuracy** and solution approach
- Identify **misleading results** and apply appropriate analyses to **judge their accuracy** or applicability

## Grading Policies

Please be aware of the following grading policies for ChE 4G03:

- 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
- The midterm and the exam will be open-book (any book) and open-notes (any hard copies), **including** any old midterms, exams, or associated solutions
- Any calculator may be used for examinations
- All grades are unofficial until final grades are posted on McMaster's student and faculty software: MOSAIC
- The instructor retains the right to modify course weights or components, typically only enforced for the student's benefit
- Final grades will be converted to the standard McMaster 12-point scale
- All submissions for assignments, 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

## Grading Breakdown

| Weight | Component | Comments |
|---|---|---|
| **0%** | Tutorial Activities | Are there to prepare you for exams, projects and assignment |
| **20%** | Assignments | 5 Assignments will count (4% each); submitted in groups of ≤ 3 |
| **20%** | Midterm Test | 2 hour written examination. May contain take-home portion |
| **25%** | Course Project | Proposal (2.5%), Report (10%), Class Presentation (12.5%) |
| **30%** | Final Exam | 2.5 hour written examination. May contain take-home portion |
| **5%** | Tutorial Participation | Attendance in tutorial sessions (0.5% each, 10 sessions) |

## Assignments

There will be 5-6 assignments for this course, each counting for 4% of the student's final grade, up to a maximum of 20%. If more than 5 assignments are released, only the best 5 results will count at 4% each. Please note the following considerations regarding the assignments:

- Assignments may be completed in groups of **up to three (3) students**
- Assignments must be submitted **electronically** to the appropriate A2L dropbox prior to the due date
- All relevant code, with appropriate comments and guidance for graders, must also be submitted with each assignment
- Assignments will typically focus on each of the five main topics of this course (broken down below), but the instructor reserves the right to modify the coverage of assignments
- All assignments will have a *demerit system* for presentation and professionalism. Any submissions that are poorly formatted, have no discussion, or show any other lack of professionalism will be penalized

## Course Project

A significant portion of the student's grade will come in the form of a course project. The project will follow a guided self-directed learning (SDL) format in which the students will develop their own topic by applying course concepts to a problem that they consider to be interesting or noteworthy. Some additional comments about the course project:

- The project **MUST** be tackled in groups of **three (3)**. *Special circumstances* will permit groups of more than three, at the discretion of the instructor
- A **proposal** (10% of project grade) will be due after approximately one month. A specific due date will be communicated by the instructor closer to the date
- After the proposal has been reviewed, each group will meet briefly with the instructor (10 minute meetings) to hammer out **specific project details and objectives**
- We will book rooms and times for **final project presentations** (50% of project grade) close to the end of the term. Each group will briefly present to a subset of the class about the problem they chose to solve, key solutions strategies and important results. Each presentation will last **15 minutes**, with a short period available at the end of the session for questions from the audience
- A **final report** (40% of project grade) detailing the problem formulation, solution methodology and results/discussion (**not to exceed 12 pages**) will be graded by the instructor

## Midterm and Exams

The course midterm (20%) and exam (30%) will primarily be written tests performed individually. As mentioned in the grade breakdown above, take-home components may be assigned depending on the interest level of the class (sometimes take-home portions for this kind of material are requested). Some other short comments:

- The final exam will be **cumulative** and may test all the components of the course
- The midterm will take place on February 26th at 7pm in MDCL 1105
- After the midterm, 1 hour of the proceeding lecture will be for reserved for a **collaborative re-write** of the same midterm in randomized groups of five (5). Your midterm score will be comprised of 85% of your individual score and 15% of your collaborative score if it is better than your individual score
- The final exam will be scheduled by the McMaster Registrar's office and will take place in early-mid April

## 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.

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. 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.

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: this point is **particularly important** and will be strongly penalized in this course
- Copying or using unauthorized aids in tests and examinations (internet-enabled devices, for example)

## Accessibility

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.

## 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 che4g3instructor@mcmaster.ca. If you would prefer to leave feedback **anonymously**, do not hesitate to use our anonymous 4G3 course feedback form.

## Dates to Remember

- First lecture: Thursday, January 09
- Reading week: Week of February 17
- Midterm exam: **Wednesday February 26** at 7pm in MDCL 1105
- Australian Open (can Roger Federer snag another major?): January 20 – February 02
- Last Lecture: April 02

## Class Recordings

As has become standard in my courses, classes will be recorded each week and posted on YouTube. Please remember that these recordings should NOT be used as an excuse to skip class, and since they are one-take I cannot make any guarantees of their availability in the event of technical difficulties.

## Anticipated Course Schedule and Topics

| Lecture Date | Anticipated Topics | Anticipated Module Content (subject to change) |
|---|---|---|
| **January 9** | Course Overview<br>Intro to Optimization<br>Formulation | • Review of course outline<br>• Concept of optimization<br>• Optimization in industry<br>• Class example – "Make the most of final year"<br>• Class workshop – "Play the game your way" |
| **January 16** | Formulation<br>Mathematical Concepts | • Types of constraints<br>• Graphical interpretations<br>• Local/Global optima<br>• Gradients and optimality<br>• Convexity and geometric interpretation<br>• Feasible directions, types of constraints |
| **January 23** | Linear Programming | • Introduction to linear programming<br>• Properties of linear programs<br>• Types of constraints<br>• Slack variables |
| **January 30** | Linear Programming | • Solution method **Simplex Search**<br>• Simplex Tableau<br>• Graphical interpretation |
| **February 6** | Linear Programming | • Sensitivity analysis/Shadow Prices<br>• Software tools |
| **February 13** | Integer Programming | • Handling of integer variables<br>• Formulating integer problems<br>• Knapsack constraints<br>• Integer relaxations |
| **February 20** | Reading Week | • Consider Richard Morgan's "Altered Carbon" |
| **February 27** | Integer Programming<br>In-class Midterm Re-Write | • Solution method: **Branch and Bound**<br>• Types of BB searches with examples |
| **March 5** | Integer Programming | • Branch and Bound continued |
| **March 12** | Unconstrained Nonlinear Programming | • **Gradient Search**<br>• **Line Search**<br>• **Golden Search** (Bisection) |
| **March 19** | Unconstrained Nonlinear Programming | • Linear relaxation<br>• Derivative-free methods (**Nelder Mead**)<br>• Quasi-Newton searches |
| **March 26** | Constrained Nonlinear Programming | • Handling constraints<br>• Penalty functions<br>• Barrier functions |
| **April 2** | Black-Box Optimization | • **Particle Swarm** Optimization<br>• **Differential Evolutions**<br>• Pros/cons of Black Box methods |