

# CHEMICAL ENGINEERING 4G03

## OPTIMIZATION IN CHEMICAL ENGINEERING

### Winter 2012 – Course Outline

**Instructor:** Kostas Apostolou (ETB 207; x20288; [apostol@mcmaster.ca](mailto:apostol@mcmaster.ca))

**Teaching Assistant:** Ali Sahlodin, JHE-370

**Schedule:**

**Lectures:** Tuesday - Friday: 8:30-9:20 JHE/326H  
**Tutorials:** T01: Monday: 9:30-11:20 JHE/233A  
T02: Monday: 14:30-16:20 JHE/233A

Total hours per week: 4 contact hours. Generally, we will use lecture time to introduce new material and solve sample problems. Tutorial time will be used for problem solving exercises and tests.

**Calendar Description:**

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 sufficient details on existing algorithms and software to solve problems.

**Objectives:**

This course will provide the student with the ability to formulate, solve and interpret meaningful optimization problems in engineering, science and business. Emphasis will be placed on the formulation of mathematical models for use with commonly available solution techniques. Software packages will be used for solving realistic engineering problems.

**Prerequisites:**

CHEM ENG 3E04, 3G04, 3M04, 3O04, 3P04

**Required Text:**

Rardin, R., "Optimization in Operations Research", Prentice-Hall, Upper Saddle River (NJ), 1998

**Web Page for Course:**

<http://avenue.mcmaster.ca/>

**Recommended Reading:**

- Edgar, T., D. Himmelblau, and L. Lasdon, "Optimization of Chemical Processes", McGraw-Hill, New York, 2001
- Reklaitis, G. V., A. Ravindran, and K. Ragsdell, "Engineering Optimization – Methods and Applications", Wiley, New York, 1983
- Williams, H. P., "Model Building in Mathematical Programming", 3rd Ed., Wiley, New York, 1990

**Software:**

- GAMS, the General Algebraic Modeling System, will be used for solving practical problems (see <http://www.gams.com/>). A student version of GAMS, with limited capabilities, can be downloaded to your personal computer at no cost. A professional version of GAMS will also be made available on the Chemical Engineering computing system for use during the course projects; this software has been donated for your use by the owner, GAMS Development Corporation
- Some problems will be also solved using MatLab and its Optimization Toolbox. These are available through the computer clusters in JHE 233/234. Students are also recommended to purchase MatLab Student Edition, which includes the Optimization Toolbox.

**Assessment:**

- Assignments (including graded tutorials) 25%
- Mid-term Exam 20%
- Course Project 25%
- Final Exam 30%

**Notes:**

- Grading will include contributions for clarity and organization of presentation.
- Up to 10 graded assignments/tutorials will be given. Graded assignments will only be accepted for up to 2 work days after the due date, with penalties of 20% and 40%, respectively. After students have submitted their papers, the solutions will be posted on Avenue 2 Learn.
- The final percentage grades will be converted to letter grades using the Registrar's recommended procedure. Adjustment to the final grades may be done at the discretion of the instructor.
- Use of only the McMaster Standard calculator during tests is allowed.

## Tentative Course Schedule

Week of	Topic	Reading
<b>I. Introduction to Optimization</b>		
Jan 2	Introduction to concepts and course	
Jan 9	Formulating an optimization problem Mathematical concepts for optimization	Ch 1-2 Ch 3
<b>II. Linear Programming (LP)</b>		
Jan 16	Principles and Concepts	Ch 5.1-5.2
Jan 23	Simplex search for LP	Ch 5.3- 5.8
Jan 30	Sensitivity in LP Special LP model formulations	Ch 7 Ch 4
<b>III. Mixed Integer Linear Programming (MILP)</b>		
Feb 6	Concepts and formulations Branch-and-bound solution method	Ch 11 Ch 12.1-12.4
<b>IV. Unconstrained Nonlinear Optimization</b>		
Feb 13	Concepts for unconstrained optimization	Ch 13.1, 13.3-13.4
Feb 20	<i>Reading week</i>	
Feb 27	One-dimensional search	Ch 13.2
Mar 6	Multidimensional search: gradient free	Ch 13.8
Mar 13	Multidimensional search: gradient based	Ch 13.5-13.7
<b>V. Constraint Nonlinear Optimization (NLP)</b>		
Mar 20	Concepts for constrained optimization	Ch 14.1-14.4
Mar 27	Constrained NLP methods	Ch 14.5-14.7
Apr 3	Sensitivity and numerical issues	

**Important Dates** (*subject to change*):

- Project proposals due: Jan 24
- Mid-term Exam: Feb 13
- Project presentations: Last week of classes
- Projects due: April 4, 16:00

## SENATE AND THE FACULTY OF ENGINEERING POLICY

### **No Adverse Discrimination**

The Faculty of Engineering is concerned with ensuring an environment that is free of all adverse discrimination. If there is a problem, that cannot be resolved by discussion among the persons concerned, individuals are reminded that they should contact the Department Chair, the Sexual Harassment Officer or the Human Rights Consultant, as soon as possible.

### **Academic Integrity**

Academic dishonesty consists of misrepresentation by deception or by other fraudulent means and 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 kinds of academic dishonesty please refer to the Academic Integrity Policy, specifically Appendix 3, located at

<http://www.mcmaster.ca/policy/Students-AcademicStudies/AcademicIntegrity.pdf>

The following illustrates only three forms of academic dishonesty:

1. Plagiarism, e.g. the submission of work that is not one's own or for which other credit has been obtained.
2. Improper collaboration in group work. Note that in this course, some tutorials and projects will be performed in groups. The group will submit one paper. All members must contribute to the paper to receive credit for the paper; therefore, the name of the group and the names of all group members who contributed to the assignment must be on the cover document. Reporting only "Group ###" is not acceptable. Placing the name of a member who did not contribute constitutes academic dishonesty for all group members.
3. Copying or using unauthorized aids in tests and examinations.

### **Changes to this outline**

The instructor and university reserve the right to modify elements of the course during the term. The university may change the dates and deadlines for any or all courses in extreme circumstances. If either type of modification becomes necessary, reasonable notice and communication with the students will be given with explanation and the opportunity to comment on changes. It is the responsibility of the student to check their McMaster email and course websites weekly during the term and to note any changes.