CHEM ENG 752 – OPTIMIZATION OF CHEMICAL PROCESSES
Term I, 2020-21 (September–December 2020)

Instructor: Dr. C.L.E. Swartz, JHE-360, Ext. 27945, swartzc@mcmaster.ca

Lectures: Provisional schedule: Tues, 9-11am; Thurs 9-10am. Lectures online via Teams. First class: Tues Sept 8, 2020.

Overview and Objectives:

Optimization is a central theme that impacts most areas of process systems engineering including process design, process control, process operations and scheduling, and parameter estimation. The primary goals of this course are to provide an overview of state-of-the-art optimization algorithms, the theoretical principles that underpin them, and their use for solving several types of practically relevant optimization problems arising in process systems engineering. The course will also cover aspects of numerical computation (such as the solution of systems of nonlinear algebraic equations, solution of initial-value ODE/DAE problems, and orthogonal collocation on finite elements) that would be useful in many areas of process engineering. Course assignments will include analysis, hand calculations, problem formulation, and solution of optimization problems of various types using different computing environments (Excel, Matlab, GAMS/AMPL) and state-of-the-art commercial grade optimization software.

Assessment:	Assignments:	65%
	Project :	35%

Reference Texts (Available in Thode Library):

I - Optimization

Biegler, L.T., *Nonlinear Programming: Concepts, Algorithms, and Applications to Chemical Processes*, SIAM, 2010.

Chvatal, V., *Linear Programming*, Freeman, New York, 1983.

Edgar, T.F. and D.M. Himmelblau and L.S. Lasdon, *Optimization of Chemical Processes*, 2nd Edn., McGraw-Hill, 2001.

Ferris, M.C., Mangasarian, O.L., Wright, S.J., *Linear Programming with Matlab*, SIAM, 2007.

Griva, I., Nash, S.G., Sofer, A., *Linear and Nonlinear Optimization*, 2nd Edn., SIAM, 2009.

Luenberger, D.G. and Ye, Y., *Linear and Nonlinear Programming*, 3rd Edn., Springer, 2008.

Nocedal, J. and S. J. Wright, *Numerical Optimization*, Springer, 1999.

Peressini, A.L., F.E. Sullivan and J.J. Uhl, *The Mathematics of Nonlinear Programming*, Springer-Verlag, 1988.

Ravindran, A., Ragsdell, K.M., Reklaitis, G.V., *Engineering Optimization*, 2nd Edn., Wiley, 2006.

Winston, W.L., *Operations Research: Applications and Algorithms*, 4th Edn., Duxbury Press, 2004.

Wright, S.J., *Primal-Dual Interior-Point Methods*, SIAM, 1997.

II – Numerical Methods

Burden, R.L., Faires, J.D., Reynolds, A.C., *Numerical Analysis*, 2nd Edn., PWS Publishers, 1981.

Conte, S.D., and de Boor, C., *Elementary Numerical Analysis*, 3rd Edn., McGraw-Hill, 1980.

PROVISIONAL COURSE OUTLINE

1. Fundamentals/Mathematical Preliminaries
   - Overview and optimization applications in process systems engineering
   - Linear equation systems and matrix factorization
   - Vector and matrix norms; condition number

2. Linear Programming
   - Fundamental theorem of Linear Programming
   - Simplex method
   - Sensitivity analysis
   - Implementation/computational issues

3. Optimization Software Environments
   - Spreadsheets
   - Low-level programming
   - Modeling languages

4. Solution of Nonlinear Algebraic Equation Systems
   - Newton's method
   - Rates of convergence

5. Optimization Fundamentals
   - Concepts and definitions
   - Convexity

6. Unconstrained Optimization
   - Optimality criteria
   - Direct search methods
   - Descent directions and line search strategies
   - Steepest descent, Newton and quasi-Newton methods

7. Constrained, Nonlinear Optimization
   - Optimality criteria
   - Sequential quadratic programming (SQP)
   - Generalized reduced gradient (GRG) method
   - Barrier/interior-point (IP) methods

8. Dynamic Optimization
   - Numerical solution of ODE and DAE initial-value problems
   - Sequential solution, sensitivity equations
   - Simultaneous approach, orthogonal collocation on finite elements

9. Mixed-Integer Programming
    - Branch-and-bound paradigm
    - Mixed-integer linear programming (MILP)
    - Mixed-integer nonlinear programming (MINLP)
    - MIP formulation issues
    - Process systems engineering applications

10. Optimization Under Uncertainty
    - Two-stage stochastic programming
    - Monte Carlo sampling
    - Chance constraints

11. Global Optimization
    - Deterministic strategies (branch-and-bound based)
    - Metaheuristic methods (Genetic algorithms, Simulated annealing)

12. Selection from
    - Mixed-integer dynamic optimization (MIDO)
    - Parametric programming
    - Mathematical programs with complementarity constraints (MPCCs)

13. Project presentations

POLICY REMINDERS:

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.

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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.

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EXTREME CIRCUMSTANCES

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