

ECH 6840

**Mathematical Methods for
Chemical Engineering**

Fall 2011

Instructor: Prof. Aydin K. Sunol
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Time and Location: TTH 12:30 - 1:45 PM NES 104
Office Hours: 2-3 PM (exclusively for the course)

Text: **Required:** “Numerical Methods for Chemical Engineering: Application in Matlab” Kenneth J. Beers, Cambridge, 2007

Recommended: “Applied Mathematics and Modeling for Chemical Engineers” Rice and Do, Wiley, 1995

Objectives: **The main objective of the course is to enable deeper level of understanding of chemical and physical changes matter undergoes through mathematical modeling and analysis.**

The objective could be achieved through mechanistic modeling, knowledge of numerical and analytical methods of solving such models, and familiarity with computational tools.

Grading Policy: (A⁺ to F)

Midterms (3)	In class 10 % (each)
	Take-Home 20 % (each)
Homework	10 %

List of Topics and Outline

Course Preview (1 lecture, Aug 23)

Modeling (2 Lectures Aug 25, 30)

Vectors and Matrices (2 Lectures, Sep 1, 6)

Solution of Algebraic sets of equations (2 Lectures, Sep 8, 15)

Solution of Ordinary Differential Equations

 Analytical and Approximate Methods (2 Lecture, Sep 17, 20)

 Qualitative Analysis (1 Lecture, Sep 22)

 Numerical Methods (2 lectures, Sep 27, 29)

 Initial Value Problems

 Boundary Value Problems

Exam 1: (Oct 4 In-Class, Take Home out on Oct 4 due on Oct 11)

Optimization

 Model Formulation (1 lecture, October 6)

 Classical Optimizations Theory (1 lecture, Oct 11)

 Calculus of Variations (1 lecture, October 13)

 Numerical Methods and Parameter Estimation (2 Lectures, Oct 18, 20)

Partial Differential Equation Solution Methods

 Analytical Methods (2 lectures, Oct 25, 27)

 Numerical Methods (3 lectures, Nov 1, 3, 8)

 Finite Difference Methods

 Finite Element Methods

Exam 2: Nov 10 In-Class, Take Home out on Nov 10 due 17)

Stochastic Systems

 Probability Nov 15

 Markov Chains Nov 22

 Monte Carlo Simulation Nov 29

 Stochastic Differential Equations Dec 1

Exam 3: Take Home out Dec 1 due in Final exam; In-class Final Exam time

There will be three 4 hour sessions: Matlab (August 27), Maple (Sep 10), and Comsol (Oct 22) for you to familiarize yourself with the software.

Welcome back and Good luck