UNIVERSITY OF ARIZONA
DEPARTMENT OF CHEMICAL AND ENVIRONMENTAL ENGINEERING
CHEE 402 – Chemical Engineering Modeling
FALL 2015

Instructor: Eduardo Sáez, Harshbarger 142C
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Office hours: Posted on D2L

Textbook: Class Notes posted on D2L. Recommended book: Rice and Do (see references).

Objectives

1. To develop methodologies used in the modeling of chemical engineering processes. This includes conceptualization, formulation, solution and analysis of chemical engineering problems, with emphasis on mathematical techniques.
2. To apply mathematical methods to the solution of chemical engineering models that lead to differential equations. The methods include analytical and numerical techniques.

Program

1. Problems leading to first order ordinary differential equations
The perfectly mixed chemical reactor: mass and energy balances. Numerical solution of first order ordinary differential equations (ODEs). Batch distillation.

2. Problems leading to second order ordinary differential equations
Homogeneous ODEs: diffusion and reaction in a biofilm. Inhomogeneous ODEs: heat transfer from a nuclear fuel rod. Systems of ODEs. Nonlinear ODEs: numerical solutions of initial value problems.

3. The Laplace transform
Transient reactions in reactors in series. Properties of the Laplace transformation. The Dirac delta function. Applications. Solutions of partial differential equations (PDEs) by Laplace transformation.

4. Problems leading to partial differential equations
Leaching from a solid: separation of variables. Sturm-Liouville theory. Inhomogeneous problems: the method of superposition. Elliptic PDEs: heat conduction. Inhomogeneous PDEs: selective destruction of tumors by radiation.

5. Numerical solution of boundary value problems and partial differential equations
Finite differences for linear ODEs. Nonlinear problems. Initial and boundary value problems for PDEs.

References

Mathematical methods:

1. Rice RG and DD Do, Applied Mathematics and Modeling for Chemical Engineers, Wiley, 1995.
2. Kreyszig E, Advanced Engineering Mathematics, 8th edition, Wiley, 1999.

Matlab:

1. Attaway S, MATLAB. A Practical Introduction to Programming and Problem Solving, 2nd edition, Elsevier, 2011.
2. Palm WJ, Introduction to MATLAB for Engineers, 3rd edition, McGraw Hill, 2010.

Course Evaluation

Homeworks
There will be homework assignments approximately every week. The final homework average will correspond to 10% of the final grade.

Tests
There will be three midterm tests; each will correspond to 30% of the final grade. There will be an **optional final exam**. For those who take the final exam, the best 3 grades in the 4 exams taken will be used to calculate the final grade.

Test 1 – Monday, September 28
Test 2 – Friday, October 23
Test 3 – Friday, November 20

Test 4 (final) – Wednesday, December 16 (8-10 am)