CHE 401 Computational Methods **Date**:5-5- 2006

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Total credits: 2 Lecture Cr: 2 Lab Cr: 0 Recitation Cr: 0

Pre Req(s): CHE 302 **Co Req(s):** **Course Designation:** Required

Contribution to professional component:

Math and Basic science Cr: 1 Engineering Cr: 1 General Education Cr: 0

Catalog Data:

Application of computational techniques for solving numerical problems that arise in chemical engineering problems. Using high-level programming languages such as Fortran or MATLAB. Topics include solving systems of linear and nonlinear algebraic equations, ordinary differential equations (initial and boundary value problem) and curve fitting.

Textbook:

J. B. Riggs, *An Introduction to Numerical Methods for Chemical Engineers*, 2nd Edition, Texas Tech University Press, 1994.

Topics covered

1. Classification of process models and the corresponding types of resulting equations. (2 classes)
2. Computational errors, conditioning and stability of algorithms. (2 classes)
3. System of linear algebraic equations (LU; Jacobi and Gauss- Siedel methods) (5 classes)
4. Nonlinear algebraic equations: Bisection; Newton-Raphson; System of nonlinear equations; Roots of polynomials. (5 classes)
5. Ordinary differential equations, Initial value problem: Taylor's series methods; Euler and Runge-Kutta methods; System of ordinary differential equations; Stability; Stiffness (6 classes)
6. Ordinary differential equations, Boundary value problem: Finite-difference method; shooting methods. (4 classes)
7. Curve fitting: Linear regression; Polynomial regression; Linear transformation (4 classes)

Course Objectives	a	b	c	d	e	f	g	h	i	j	k
1. Understand why computational methods are important in modern Chemical Engineering								3	2	3	2
2. Be able to identify the appropriate problem class (nonlinear equations, ordinary differential equations, etc.) of a given a physical problem that is already in a mathematical form.					3			1	1		
3. Be able to identify, within a problem class, the appropriate solution methods.					3						
4. Be able to write algorithms and software and/or use commercial or public-domain packages for solving mathematical problems in Chemical Engineering. [1](1,2)	3										3
5. Be able to check the correctness of an algorithm, a code, and of numerical results of a calculation	3										
6. Be able to solve systems of linear algebraic	3										3