

CHE 401 Numerical Methods

Date:5-5- 2006

Instructor: AbdelHamid Ajbar

Total credits: 2

Lecture Cr: 2

Lab Cr: 0

Recitation Cr: 0

Pre Req(s): CHE 302

Co Req(s):

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)

Objectives

	a	b	c	d	e	f	g	h	i	j	k		L	M
1. Understand why computational methods are important in modern Chemical Engineering								3	2	3				
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									
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	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 equations	3										3			

