

**COMMONWEALTH GRADUATE ENGINEERING PROGRAM
DISTANCE LEARNING COURSE PLANNING SHEET
UNIVERSITY OF VIRGINIA**

Course:
Semester:
Instructor:
Phone No.:
Office Address:

E-Mail Address:

Very important to get the following information asap so that off-grounds students and sites can order books:

Textbook(s): (Student to purchase)

Reference(s): Limit 4

Computer Needs:

Computer Capability:

Software required:
Provided?

Other:

Please attach a copy of your course syllabus, biographical sketch, and any other information we might need to prepare for this course.

Chemical Engineering 665
Techniques for Chemical Engineering Analysis & Design

Tentative Syllabus
Fall 2008

I. ITERATIONS/DIFFERENCE EQUATIONS

1. Iterations/difference equations.

II. Sets of Algebraic Equations

2. Linear Algebraic Equations and Properties of Matrices.
Simultaneous Linear Equations
Rank
3. Homogeneous Linear Equations
Eigenvalues and Eigenvectors.
Singular value decomposition; general linear least squares (Numerical Recipes, p23, pp52-64, and pp 504-519).
4. Newton-Raphson method for single equations and systems of nonlinear equations (Num. Recipes, pp269-273).

III. Ordinary Differential Equations

5. Complete solution to linear ODEs. First order linear ODEs.
Sets of 1st order linear ODEs
6. Sets of 1st order linear ODEs.
7. Nonlinear ODEs: initial value problems.
8. Nonlinear ODEs: initial value problems; Numerical solution of initial value problems
9. Boundary value problems;
Bessel's Equation. Modified Bessel's Equation.
Sturm-Liouville problems and Orthogonality of functions.
10. Sine, cosine: Orthogonality and expansion of arbitrary functions in series, Fourier Integral.
Bessel functions: Orthogonality and expansion of functions..

11. Principal component analysis: reconstructing experimental data
12. Numerical solution of boundary value problems
13. Collocation methods.

IV. Partial Differential Equations

14. Classification of partial differential equations: Linear PDEs: analytical solutions
15. Separation of Variables and Finite Fourier transform
16. Separation of Variables and Finite Fourier transform
17. Quiz I (Covers I, II and III)
18. Numerical solution of PDEs—finite difference
19. Numerical solution of PDEs
20. Numerical solution of PDEs
21. Perturbation expansions
22. Perturbation expansions/intro to projects
23. Collocation methods for PDEs.
24. Final quiz
25. Reports.
26. Reports

Chemical Engineering 665
TECHNIQUES FOR CHEMICAL ENGINEERING ANALYSIS AND DESIGN
Fall 2008

COURSE OUTLINE

Catalog Description: ChE 665: Techniques for Chemical Engineering Analysis and Design (3)
Prerequisites: Undergraduate differential equations, transport processes, and chemical reaction engineering. Development of analytical and numerical methods for analysis of steady state and transient chemical engineering problems arising in fluid mechanics, heat transfer, mass transfer, kinetics, and reactor design.

Instructor: J. L. Hudson, Professor of Chemical Engineering
Office: 117F Chem. Eng.
E-mail: hudson@virginia.edu

Textbook: We shall not follow a single textbook. You should have a good applied mathematics textbook to which you can refer. The book by Varma and Morbidelli, which is listed below, is one good text. You will also need to refer to books on numerical analysis.

Copies of the lecture notes should be purchased through the UVa Bookstore. **This is not a textbook.** The notes simply contain the equations that we shall discuss; there are no accompanying words and no explanation of the equations. The notes are meant to be an aid in decreasing the amount of time spent writing down equations in class. You'll want to add your own notes during the lecture and during our discussions. We would like to use class time for discussion; so please look through the notes before class and bring your thoughts and questions.

References: Mathematical Methods in Chemical Engineering, A. Varma and M. Morbidelli, Oxford Univ. Press, New York (1997).

F. B. Hildebrand, "Advanced Calculus for Applications," 2nd edition, Prentice-Hall, 1976.

Deen, William M., "Analysis of Transport Phenomena," Oxford, 1998.
(Particularly perturbation methods, pp. 94 to 112 and solution methods for conduction and diffusion problems, chapter 4.)

Press et al., "Numerical Recipes," Cambridge University Press, 1986.

Goals: This course is intended to increase the skills of MS level students in solving the types of equations which arise in chemical engineering processes.

Prerequisite by Topic:

1. Mathematics through ordinary differential equations (initial value problems).
2. Knowledge of some computer programming language.
3. Transport operations.
4. Chemical reaction engineering.

Topics:

1. Iterations/Difference Equations
2. Algebraic equations: Matrix Methods. Eigenvalues and eigenvectors. Singular value decomposition and fitting data. Root finding.
3. Ordinary Differential Equations: Introduction to mathematical models in chemical engineering. Simultaneous ODE's. Review of initial value problems. Boundary value problems. Orthogonal functions. Principal component analysis. Numerical solution of ODE's. Artificial neural networks.
4. Partial Differential Equations: separation of variables and finite Fourier transform method. similarity transformation. Numerical solution of PDE's.
5. Perturbation Methods

Grading (tentative):	Quiz:	25%
	Final	35%
	Homework	20%
	Projects	20%

Examinations: The quizzes and the final will be closed book.

Computer programming and usage: We will be learning how to treat models of problems of interest in Chemical Engineering with the use of both analytical solutions and numerical methods. This is not a course in computer programming. Nevertheless, you will be expected to develop computer codes to solve problems. If you know a programming method such as C⁺⁺ or Fortran, then by all means use that; you may use the unix system or the PC based system. (There is a good PC based system for C⁺⁺ at the University but if you use Fortran, you will have to use the unix based system.) If you prefer, you may also use either Matlab or Visual Basic. I recommend Matlab as it is very convenient to use and most students find it to be an excellent tool. If you do use Matlab, you will be asked to write code to solve problems.

Homework policy: Late homework will normally not be accepted. Homework sets will be graded 2, 1, or 0 ---- 2 for acceptable work, 1 for conceptual errors, 0 for minimal effort. A reasonable amount of verbal collaboration among students taking this class is expected and encouraged. However, the work must be your own. Do not refer to problem solutions or computer programs from previous years. For some of the computer projects special instructions shall be given and these projects will have more weight than the normal homework assignments.

Instructor information;

Please see <<http://www.che.virginia.edu/hudson.html>>