CME 420 Process Modeling

Spring 2010
University of Kentucky College of Engineering, Paducah
Lecture: 11:00AM-12:15PM TR CLC 219
Course Web Page: http://www.engr.uky.edu/~silverdl/CME420/

INSTRUCTOR:	Dr. David L. Silverstein	
	209 Crounse Hall (270) 534-3132 (Office) SilverDL@engr.uky.edu	Office Hours: Open door policy-- when I am there, I am usually available. To guarantee availability, make an appointment.
CATALOG COURSE SUMMARY:	Applications of principles of material and energy balances, thermodynamics, heat and mass transfer, physical chemistry and numerical methods to problems in separation and transport processes and reactive systems. Prereq: CME 199, MA 214; Prereq or concur: CME 320, CME 330, engineering standing.	
TEXT:	Required: *Numerical Methods for Engineers* , Sixth Edition, Steven C. Chapra & Raymond Canale, 2002. *Problem Solving in Chemical Engineering with Numerical Methods*, Cutlip & Shacham. References: *An Introduction to Numerical Methods for Chemical Engineers*, Second Edition, J. B. Riggs, 1994; *Advanced Engineering Mathematics*, Kreysig; *Advanced Engineering Mathematics*, Lopez; *Applied Mathematics and Modeling for Chemical Engineers*, Rice & Do Other references include programming texts, texts used in Process Principles, Fluid Mechanics, Heat & Mass Transfer, Thermodynamics, Calculus I-IV. These supplementary texts are either available in the library or may be borrowed on a limited basis from the instructor.	
COURSE OBJECTIVES:	This course is designed to provide juniors in chemical engineering the tools necessary to formulate chemical engineering problems using the concepts learned in the core chemical engineering courses. In addition, various techniques for solving algebraic and differential equations are presented in this course.	
COURSE EXPECTATIONS:	At the conclusion of this course, you should be able to: 1. Model various processes using chemical engineering principles. 2. Use concepts of material and energy balances, thermodynamics, fluid dynamics, and kinetics to develop model equations. 3. Use computer software and programming languages to solve complex mathematical systems.	
COURSE POLICIES:	Attendance is expected at all lectures. Instructor reserves the right to administer unannounced quizzes on reading or lecture material during classes. Bring your calculators to all classes. Homework assignments will be distributed in class. Homework is due within the first five minutes of the scheduled start of the period for which it is assigned. Late homework will receive no credit. Homework must be submitted on 8.5"x11" green **engineering paper** (except for computer printouts), **one side** per page. All pages should be **numbered** and contain your **name**. Multiple pages should be secured by **paper clip** and not folded or stapled. Individual solutions should **stand alone--** no reference to the source of the original problem should be required to understand the context and meaning of the solution you present. Each solution should contain a **problem statement**, a list of **assumptions**, a **diagram** (if appropriate), and a solution containing **adequate steps and explanations** to ensure understanding of your solution by the instructor. The final solutions to a homework problem must be **boxed** or otherwise distinguished from the remainder of the problem. Problems solved using a computer must contain all information required to reproduce your solution. Among other things, this means a spreadsheet printout only containing numbers is not sufficient. The formulas used must be included on the printout. All numbers must be identified and labeled with appropriate units. **You must submit the data file for problems solved with computers.** Specific guidelines for completing programming problems will be provided with the first programming assignment.	

	Homework assignments are individual tasks. No copying of solutions is permitted. You are, however, encouraged to work in small groups to discuss methods of solving the homework problems. Bear in mind that setting problems up is the most difficult part of most problems, and failure to practice setting problems up independently will likely result in an inability to set problems up on exams. You must indicate whom you work with on assignments completed with assistance from a group. Certain assignments may be designated group problems and must be solved as a group. Details on group problems will be provided when assigned. Any disputes regarding grading must be resolved within 5 school days of the original issuance of the grade. Requests to re-grade a problem may result in the entire assignment being re-graded and adjustments to all scores being made. This can potentially result in a decrease of score. Any grades not challenged within the five school day period are considered final. This applies to both homework and exams. Cheating is strictly forbidden, and anyone found doing so will be turned over to the University Registrar and dealt with in accordance with University policy. Working together on homework is encouraged, but each person must independently write-up their own work and **cite any assistance they have had from classmates**. **Copying homework** (problems, graphs, figures, computer files, etc.) **between individuals is cheating.**
GRADING:	Final Exam: 30% Hour Exams 45% Homework Assignments/Quizzes: 25% A weighted grade of 90 or above is guaranteed an A, 80 or above at least a B, 70 or above at least a C, and 60 or above at least a D. A grade of E will be assigned to anyone earning a weighted grade below 60. For grades near the endpoints in the above distribution, consideration will be given to homework performance, class participation, and performance trends as a function of time. Homework and exam problems will be graded based on the following factors: correct assumptions, correct diagrams, legibility, clarity, neatness, identification of paper, clearly defined answer, correct approach to problem, and the correct answer. These criteria will be weighted according to the instructor's judgment for a particular problem. Satisfactory completion of homework may be required to pass the course.
COURSE CONTENTS:	1. Computers and Numerical Methods A. Numerical Error B. Taylor Series Approximations 2. Fundamentals of Modeling 3. Solution of Algebraic Equations A. Single and Systems of Nonlinear Equations B. Systems of Linear Equations 4. Linear and Nonlinear Regression A. Linearizing Equations B. Linear Regression C. Multiple Linear Regression D. Nonlinear Regression 5. Polynomial Approximations A. Finite Difference Approximations B. Interpolation C. Integration 6. Optimization A. Maxima and Minima B. Lagrange Method of Undetermined Multipliers 7. Ordinary Differential Equations A. Analytical Solution of First and Second Order Linear Differential Equations B. Numerical Solutions C. Solution of Systems of Ordinary Differential Equations Specific topics are subject to medication at instructor's discretion. Extensive examples of applications to chemical engineering problems will be covered for each topic.

HOMEWORK:	Approximately 15 assignments will be given. Some homework assignments will require use of a computer software package. Unless otherwise specified, any suitable software package may be used to complete your homework (Maple, MathCAD, MATLAB, C/C++, FORTRAN, Visual BASIC, Polymath, spreadsheet).
EXAMINATIONS:	There will three in-class examinations and a final examination. The in-class exams will be cumulative since the previous exam. No make-up hour exams will be given except with the advance consent of the instructor. The final exam will be comprehensive. There will be no make-up final exam. Exam dates are February 11, 2010; March 11, 2010; April 22, 2010. These dates may be changed by mutual consent with at least one week warning. The Final Exam will last 2.5 hours and will begin at 10:45AM on Tuesday, May 4, 2010. The date and time for this exam is set administratively and cannot be changed.
FIRE SAFETY:	In the event of a fire, all students, faculty and staff should leave the building through the nearest exit and gather in the parking lot in front of Crounse Hall. A fire alarm should be treated as indicative of an actual fire.
INCLEMENT WEATHER:	WKCTC Snow day policy will be followed for this class. If start of classes is delayed due to inclement weather, this class will start at 12:00 PM. Information on delayed class start or campus closure will be broadcast over WPSD-TV and over radio by WKYQ-WKYX, WDDJ, WDXR, WNGO-WXID (Mayfield), WCBL (Benton), WMOK-WREZ (Paducah-Metropolis), and WKMS (Murray).

Course Schedule

Period	Date	Reading Assignment	Problems Due
Lecture	01/12	Chapters 1-3 (Basics of Modeling)	
Lecture	01/14	Chapter 4 Taylor Series	
Lecture	01/19		Problem Set #1
Lecture	01/21	Chapter 5-8 (Roots of Equations)	
Lecture	01/26		Problem Set #2
Lecture	01/28		
Lecture	02/02	Chapters 9-12 (Linear Algebraic Eq.)	Problem Set #3
Lecture	02/04		
Lecture	02/09		Problem Set #4
EXAM	02/11	Exam 1	
Lecture	02/16	Chapters 17-20 (Curve Fitting/Interp.)	Problem Set #5
Lecture	02/18	Regression	
Lecture	02/23	Interpolation	Problem Set #5
Lecture	02/25	Chapters 21-24 (Numerical Int./Diff.)	
Lecture	03/02		Problem Set #7
Lecture	03/04	Chapters 13-16 (Optimization)	
Lecture	03/09		Problem Set #8
EXAM	03/11	Exam 2	
Holiday	03/16	Spring Break	
Holiday	03/18	Spring Break	
Lecture	03/23	Unsteady-state balances (FR)	Problem Set #9
Lecture	03/25	Chapters 25-28 (ODE)	
Lecture	03/30	Analytical Methods	Problem Set #10
Lecture	04/01		
Lecture	04/06		Problem Set #11
Lecture	04/08	Numerical Approaches	
Lecture	04/13		Problem Set #12
Lecture	04/15	Boundary Value Problems	
Lecture	04/20		Problem Set #13
EXAM	04/22	Exam 3	
Lecture	04/27	Simulation and Modeling	Problem Set #14
Lecture	04/29	Process Simulators	Problem Set #15
Final Exam	05/04	Comprehensive Final Examination	10:45 AM - 1:15 PM

All material on this schedule is subject to change at instructor's discretion for pedagogical reasons.