University of Kentucky
Chemical and Materials Engineering Department

EGR 199-001: Computational Tools for Chemical Engineering
Spring 2007

Instructor: Dr. Stephen Rankin
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Office hours: TBA, or by appointment

Time and Place: Tuesday 2:00 - 2:50 pm, FPAT [F.P. Anderson Tower] 263
Thursday 2:00 - 2:50 pm, BE [Business and Economics] 105

Teaching assistant: TBA
Office hour: TBA
e-mail: TBA

Textbook: Prentice Hall compilation of chapters from R. W. Larsen, Engineering with Excel
The textbook in the bookstore contains excerpts from all books [ISBN 0536878811].

Course web site: http://www.engr.uky.edu/~srankin/egr199.htm - this will be replaced with
a Blackboard site as soon as possible – to learn about Blackboard, go here:
http://www.uky.edu/IT/CustomerService/docs/blackboard

Prerequisite: Enrollment in college of engineering, or permission of instructor.

Course description
Throughout the chemical engineering curriculum at the University of Kentucky,
computational tools are used to solve complex problems. This course will serve as an
introduction to those tools, and to basic computer programming concepts that allow the efficient
solution of engineering problems. The programs that will be emphasized include Microsoft
Excel, visual BASIC for applications (VBA) and Maple.

Objectives: By the end of the course, students should:
1. Develop proficiency with spreadsheet calculations and graphing with Microsoft Excel
2. Understand and be able to use the Maple user interface to solve equations and systems of
equations
3. Know the basic capabilities Excel and Maple, and know when to apply them
4. Be able to perform linear regression for a set of data
5. Understand basic concepts of computer programming such as decision statements and
constructing loops
6. Write simple visual basic programs to solve engineering problems
7. Be able to numerically solve nonlinear equations using Maple and Excel
8. Be able to numerically solve sets of linear equations using Maple and Excel
Important Dates

January 11  First day of class.
February 20  Exam 1
March 5       Midterm of semester.
March 13 & 15 Spring break. No class.
April 5       Exam 2
April 26      Last day of class.
May 3         Final Exam, 1:00-3:00 pm

Grading

The following percentages will guarantee that a student receives that grade. If the average for the class warrants adjusting the grade distribution, the grade cutoffs may be adjusted, always in favor of higher grades.

100% to 90%: A  89% to 80%: B  79% to 70%: C  69% to 60%: D  <60%: E

Grades will be assigned for individual assignments based on this scale, but at the end, all scores will be added together and weighted according to the components specified below, to determine the final grade. If a student receives a “D” or “E” on all exams and quizzes, homework and group project grade (see below) will not be counted (and the score will be renormalized).

Grading Components

<table>
<thead>
<tr>
<th>Component</th>
<th>Percentage</th>
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<tbody>
<tr>
<td>Final Exam</td>
<td>35%</td>
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<tr>
<td>Exams (2)</td>
<td>15% each</td>
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<tr>
<td>Quizzes</td>
<td>15%</td>
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<tr>
<td>In-class assignments</td>
<td>10%</td>
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<tr>
<td>Homework</td>
<td>10%</td>
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Computer Hardware, Software, and Accounts

This course requires the use of a computer to receive assignments and announcements as well as to complete assignments. The University of Kentucky provides a large number of computing facilities to students, all of which have the software required for this course. For a complete list of facilities, visit the student computing services web site (http://www.uky.edu/SCS/labs). Students do not need to purchase any software. The University also provides students with the accounts. Freshman who enrolled in 2006 should automatically have an active directory (AD) account that has the same user name and password as their official UK e-mail. Students will need to use that user name to log into Blackboard, and official course announcements will be sent to uky.edu e-mail addresses. To check the status of your account, go to http://u-connect.uky.edu. If students choose to use another e-mail address, they must forward their e-mail from the uky.edu server (you can learn how from the u-connect web site).

Discussion Board

To facilitate discussion and to give the students more opportunities to ask questions, a discussion board will be set up on Blackboard. Students are encouraged to use the discussion board to ask questions, and to discuss / answer each other’s questions. The forum will be monitored by the instructor, and inappropriate content will be removed. This includes comments
that do not show appropriate respect for other students or direct posting of the final answers to questions (such as “The answer to question 3 is 3.14”). The focus of the discussion should be more on the methods to solve problems rather than the answers.

**Reading, Homework, and Learning Strategies**

Reading assignments will be posted on the course web / Blackboard site and announced in advance in class. You will make the best use of your time in class if you keep up with the assignments, and come prepared for class. You may have an easier time doing the homework if you review the reading and notes before starting. This will be particularly important in this course, because we only meet twice a week, and one of the class sessions is devoted to in-class computer labs.

**In-class Computer Assignments**

On Thursdays, we will meet in a computer lab in the B&E building (see above). Some of the time will be spent on in-class assignments that will need to be turned in by the end of class (they will need to be e-mailed to the TA). Sometimes quizzes will be held instead, which will also need to be turned in by the end of the class period and will contribute more to the student’s grade. Because there will be a time limit on the assignments, it is important that students come prepared, and have practiced either by reading and following with the assigned reading, or by doing the assigned homework. There also will sometimes be quizzes that need to be completed before classes using the Blackboard system (these will be announced in class and on the Blackboard announcements page).

**Attendance**

Attending classes is highly recommended, and will be necessary on Thursdays to complete in-class assignments and quizzes.

**Academic Integrity**

All work that students turn in will be expected to be their own. Due to its digital nature, the temptation to copy computer files may be greater than handwritten work. However, instances of cheating and plagiarism will be taken very seriously in this class. Students will be asked to e-mail their answers to in-class exercises and some homework problems, to reduce the possibility for copying without detection. Students found to violate principles of academic integrity will at least receive an “E” for the course.

**Tentative Sequence of Topics**

It will be important to check the course web / Blackboard site occasionally for changes in the timing and sequence of covering these topics, but the tentative sequence will be:

A. **Excel basics**  
   a. Introduction to spreadsheets and Excel [Larsen Ch. 1]  
   b. Plotting with Excel [Larsen Ch. 2]  
   c. Excel functions [Larsen Ch. 3]

B. **Linear regression in Excel**  
   a. The linear regression problem  
   b. Excel’s trendlines – use and interpretation [Larsen Ch. 5]
C. Solving nonlinear equations
   a. Approaches to solution [Larsen Ch. 6]
   b. Newton-Raphson method
   c. Implementing Newton-Raphson method in Excel

D. Macros and VBA
   a. Using Macros in Excel to automate tasks [Larsen Ch. 7]
   b. Introduction to VBA and modular programming [Chapra Ch. 1-2 and 5]
   c. Writing and debugging programs [Chapra Ch. 7]
   d. Data types, variables and functions in VBA [Chapra Ch. 8-9]
   e. Structured programming: decisions [Chapra Ch. 11]
   f. Structured programming: loops [Chapra Ch. 12]
   g. Data structures and file operations in VBA [Chapra Ch. 13-14]

E. Maple basics
   a. Introduction to user interface and syntax [Schwartz Ch. 1-6]
   b. Plotting functions in Maple [Schwartz Ch. 8]

F. Sets of Linear Equations
   a. Matrix representation of set of equations
   b. Matrix operations in Excel (inversion approach) [Larsen Ch. 4]
   c. Gaussian elimination in Excel with VBA
   d. Matrix algebra in Maple [Schwartz Ch. 10]