Ch.E. 375, Computer Tools/Skills in Chemical Engineering, W, '09
Section A: T 11:30-1:30, 2 credits
Section B: W, 1:30-3:30, 2 credits

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During your career in the Department of Chemical Engineering, you will find it necessary to use computer programs such as Excel, MATLAB, Simulink, AspenPlus, and Comsol Multiphysics, which used to be called FEMLAB. These tools allow you to study realistic problems and explore alternatives that would be inaccessible if you had to do the computations yourself. However, some effort is required to use the computer tools. This course will reinforce your use of Excel, and teach you the basics of MATLAB, AspenPlus, and Comsol Multiphysics. Simulink is covered in Ch.E. 480. The course is an elective and counts towards technical electives or free electives.

The course is structured around the types of problems you are being asked to solve Winter quarter, have solved in the previous Autumn quarter, and will solve in Spring quarter. It is hoped that by focusing on activities that are close in time your motivation will be higher. The course meets one hour per week in lecture, followed by one hour in the computer lab.

Typical problems include:
- Solving a single nonlinear equation in one variable (cubic equation of state for multi-component thermodynamics), CHEM E 310, 326;
- Solving sets of nonlinear equations (chemical equilibrium or phase equilibria), CHEM 326;
- Solving recycle problems in Excel and Aspen, CHEM E 310;
- Plotting the results in Excel, MATLAB, Aspen, and Comsol Multiphysics;
- Solving initial value problems (tank drainage and heat transfer), CHEM E 436 and 340;
- Solving two point boundary value problems in Comsol Multiphysics, CHEM E 330 and 340;
- Solving partial differential equations in Comsol Multiphysics, CHEM E 330 and 340.

For each topic, the lecture hour will outline the method used to solve a class of problems, and will give specific techniques to be used in doing so. A handout will give the details each week. Then in the laboratory hour following, you will can work in pairs or by yourself to solve a problem like those solved in class. In this hour you will have a chance to apply the techniques, and solve an interesting chemical engineering problem with lots of help. The laboratory problem is not turned in, and group work is allowed and encouraged. After the laboratory, a problem of the same type is assigned that is to be solved **on your own**. This problem will be turned in Friday or Monday (for T and W section, respectively), and the papers will be returned in class. If you were unsuccessful, corrections and suggestions will be given so that you can redo the problem and get it right. This is similar to real engineering work - you have to do it and redo it until it is right. No one wants the bridge to fall down or the reactor to explode. Thus, assignments will be given credit once they are correct – there is no partial credit. But, you will have a chance to redo

them. Also, you must show how you checked your computer work before credit is given. This is similar to what you'd do on the job: your supervisor wants to know why you think the answer is correct. He/she gives no partial credit, and the correct result is expected.

Credit will be given to those students (a) attending the lectures and laboratories and (b) turning in successful assignments of 9 of the 10 assignments. The assignments turned in should be your own work. The penalty for turning in someone else's work as your own is loss of credit for that assignment.

Textbooks

The textbook is: Introduction to Chemical Engineering Computing, by Bruce Finlayson.

Schedule (including the programs used that week or later weeks)

Week 1: Jan. 5-11: Equations of state; nonlinear equations of one variable; virial equation with Leonard-Jones potential; Excel, MATLAB, AspenPlus.

Week 2: Jan. 12-18: Phase equilibrium; nonlinear equations; Excel, MATLAB, AspenPlus.

Week 3: Jan. 19-25: Chemical equilibrium; nonlinear equations; chemical equilibrium based on molecular parameters; Excel, MATLAB, and AspenPlus.

Week 4: Jan. 26-Feb. 1: Mass balance with recycle, including chemical equilibrium; nonlinear equations; Excel.

Week 5: Feb. 2-8: Simple units; ASPEN.

Week 6: Feb. 9-15: Complicated units with recycle; ASPEN.
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Week 7: Feb. 16-22: Chemical reactors; ordinary differential equations; MATLAB

Week 8: Feb. 23-Mar. 1: Flow/heat transfer; boundary value problems; Comsol Multiphysics.

Week 9: Mar. 2-8: 2D flow; molecular motion; Comsol Multiphysics.

Week 10: Mar. 9-15: 2D flow and diffusion; microfluidics; Comsol Multiphysics.