CM3450

Computer Aided Problem Solving

Instructors: Dr. Tom Co (tbco@mtu.edu) and Dr. Tony Rogers (tnrogers@mtu.edu)

Scheduled Time and Room: MWF, 1-3pm, MEEM 120

Class Homepage: www.chem.mtu.edu/~tbco/cm3450/cm3450_2k8.html

Required Text:

Heranto Adidharma and Valery Temyanko, **Mathcad for Chemical Engineers**, Trafford Publishing, Victoria, Canada, 2007.

Other References:

Michael B. Cutlip and Mordechai Sacham, Problem Solving in Chemical and Biochemical Engineering with Polymath, Excel and Matlab, 2nd Edition, Prentice Hall, Boston, MA, 2008.

UniSim R380 online documentation (available through the link: P:\UniSim\R380\Documentation\USD\UniSim Design Menu.pdf)

Objectives: To attain the basic skills and understanding of the methods and advanced techniques of using computers for the solution and analysis of complex chemical engineering problems and applications.

Grading:

Weekly Assignments	35 %
Projects	50 %
In-class Tasks/Portfolio	15 %

A	95-100
AB	90-94.99
B	85-89.99
BC	80-84.99
C	75-79.99
CD	70-74.99
D	60-69.99
F	0-59.99

Additional Policies:

1. It is strongly suggested to have a bound (composition) notebook dedicated for the class to jot down tips, ideas and problems.
2. A binder is required to collect and organize assignments and projects.
3. Attendance is required for the Monday and Wednesday classes. The Friday class will be problem solving/consultation sessions only. Letters need to be submitted formally and officially to request for excused absences, and it should include: date, reason, documentation and plan for makeup. Valid reasons include: sickness, job interviews, athletic, university or military obligations.
4. Assignments and projects need to be done individually. Discussions are allowed but the work can not be copied (revising another student's document is not allowed). Each submission should be attached with a signed cover letter that includes the following statement:

   " I have done this work on my own."

   If you did discuss with other students then please attach the following information:

   "I discussed the assignment/project only with (…names of persons…)"

5. Late submissions of assignments and projects will be deducted 10 points a day.

6. Projects should be submitted with a formal memo report that:
   a. Identifies all assumptions used
   b. Discusses clearly the procedure used
   c. Summarizes the results and findings
   d. Clearly addresses the requested items
   e. Includes all supporting materials such as references and printouts (in an appendix).
7. Weekly assignments should be submitted as a one-page memo report (hardcopy) together with attachments of the programs or files (which could be sent by email).

Course Syllabus

Microsoft Excel Spreadsheet (T. Co)

Week 1

Data tables
Successive Subsitution (lecture)
Arrays and array functions
Solution of Simultaneous Linear Equations

Week 2

Linear Regression
SOLVER – Solution of Equation
SOLVER – Optimization and Nonlinear Regression

Week 3

VBA Programming
- Functions and Subroutines
- User Interface and Controls

Advanced topics
- Newton Raphson (lecture)
- Runge-Kutta (lecture)

MathCad (T. Co)

Week 4

Basics of MathCad
- Equations, Units and Functions
- Plotting, Data Export/Import

Week 5

Solution of Nonlinear Equations
- "Roots" function and "Find" blocks
- Parameterization of initial guesses

Week 6

Symbolic Manipulation
- Menu operations
- "Live" symbolic mode

Numerical Differentiation and Integration

Week 7

Optimization – unconstrained and constrained
Basics of MathCad Programming – creating functions

MatLAB (T. Co)

Week 8

Basic operations
Linear Solvers – sparse matrix approaches

Week 9

Programming – m-script files, m-functions
ODESolvers

Week 10

Multidimensional Arrays and Structures
Plotting and Animation

Week 11

Introduction to Simulink

UniSim (T. Rogers)

Week 12 - Basics of UniSim

1. Setting global simulation 'Preferences'
2. Configuring the "Basis Environment"
   - Components
   - Thermodynamics models
   - Reaction sets
3. Building a process flowsheet
4. Results & Reporting
5. Assign Project #3

Week 13 - UniSim 'Simulation Environment'

1. Recycle Block
2. Adjust Block
3. Unit Operations 'Palette'
4. Degrees of freedom for user inputs
5. Specifying subcooled, saturated, and superheated streams
6. Rankine steam power cycle example

Week 14 - More UniSim Examples & amp; Tips

1. Reactors (CSTR, PFR, Equilibrium, Conversion)
2. Phase Separators (2-phase, 3-phase)
3. Mixers & Tees
4. Staged Separations (Distillation Columns, Absorbers, Strippers)