University of Texas-Austin - Integration of Computing

During 2001-2002 the Department of Chemical Engineering at UT-Austin revamped the computing thread in its curriculum in order to strengthen student background in computing. This action was in response to student and faculty dissatisfaction with the depth and continuity of computer training over the four years of the program. The curriculum modifications included:

1. Adding a new ChE freshman course, ChE 210: Introduction to Computing, focusing on basics of computing, MATLAB, and Excel.

2. Changing ChE 448 to ChE 348 to focus on Numerical Methods in Chemical Engineering and Problem Solving, in the second semester – sophomore year.

3. Changing the existing junior lab course (3 credit hours to two two-credit hour courses: ChE253K: Introduction to Statistics and Data Analysis, and ChE 253M, Fundamental Measurements Laboratory.

In addition, reinforcement of the computing tools was implemented in core ChE courses by identifying prototype problems where these tools (mostly Excel and MATLAB) would be used. Table B.1 shows the layout of the required courses and where computing is employed.

Table B.1. Computing Tools Used in the ChE Curricula at UT-Austin

Year	Computing Activities
Freshman	Introduction to MATLAB, Excel (second semester)
Sophomore	Material and Energy Balances (Excel) Numerical Methods (MATLAB, Excel) Transport Phenomena (Excel)
Junior	Thermodynamics (Excel) Fluid Flow/Heat Transfer (MATLAB, CFD) Statistics (JMP, Excel) Separations (Aspen, Excel) Measurements Laboratory (JMP, Excel)
Senior	Reactor Design (MATLAB, Excel) Process Control (MATLAB, Excel) Unit Operations Laboratory (data acquisition/control, Excel) Process Design (Aspen, @Risk, Excel)

The advantage of the proposed changes is that computing and numerical analysis are now spread uniformly over the first three years of the program, namely two hours on

computer software tools in the second semester of the freshman year (ChE 210), three hours of numerical analysis in the second semester of the sophomore year (ChE 348), and two hours of statistics in the third year, increasing statistics instruction from one hour to two hours (ChE 253K). The doubling of coverage of statistics was in response to feedback from industry on the importance of statistics in chemical engineering practice. Note that even with all of these changes, there was no net increase in the number of credit hours for the degree.

The objectives of the two modified computing courses (210, 348) are as follows. Upon completion of ChE 210 students should:

- Understand basic computer architecture and internal number representation.
- Have an appreciation for limitations in numerical accuracy.
- Be able to construct plots, fit data, and build new functions using Microsoft Excel.
- Demonstrate ability to create complex programs in a programming environment such as MATLAB.

Upon completion of ChE 348 students should:

- Be able to identify and formulate methods to solve specific classes of numerical problems, including linear equations, nonlinear equations, numerical integration (quadrature), least-squares curve-fitting, minimization of functions, and differential equations.
- Understand how software can be used to solve each class of problem.
- Know limitations of each method.

Detailed outlines of the three new/revised courses (210, 348, 253K) are given below. For each topic, the number of one-hour lectures are given in parentheses.

ChE 210 (Introduction to Computing)

1. Introduction to Computers (5)
   - History of computing devices
   - Modern computer architecture
   - Number representation and round-off
   - Internet, web, HTML

2. Spreadsheets (7)
   - Simple cell arithmetic
   - Plotting data – data visualization – good graphics
   - Solver
   - Visual Basic for applications

3. Programming Concepts (9)
   - Problem analysis and specification
   - Algorithms and control structures
   - Flow Charts and pseudocode
   - Sequential processing (order of precedence, arithmetic operations)
   - Selection structures (if-end, if-else-end, if-else if-else-end)
   - Repetition structures (for, while)
   - Comparison operators and Boolean expressions

4. MATLAB Programming (8)
   - Matrices and vectors
   - Plotting
   - Scripts
   - Functions
   - Selection, repetition and logicals

ChE 348 (Numerical Analysis)

1. Review of Program Organization and Structure (4)
   - Overview of course and MATLAB
   - Review of programming, control structures
   - Review of Taylor series
   - Errors, accuracy and stability

2. Matrices (3)
   - Elementary matrix-vector operations
   - Properties of matrix operations: eigenvalues, diagonalization
   - MATLAB operations

3. Linear equations (3)
   - Gaussian elimination/partial pivoting
   - Tridiagonal and band diagonal matrices

4. Single Nonlinear Equations (3)
   - Graphical solution
   - Newton, secant, Broyden methods

5. Multiple Nonlinear Equations (5)
   - Graphing zero contours
   - Newton's method, partial derivatives
   - MATLAB: fsolve
   - Example: Multiple reactions, CSTR

6. Differential Equations (7)
   - Review of ODE's: linear vs. nonlinear ODE's, order of ODE's, linear first order ODE's (integrating factors), and solutions of second order ODE's.

Quadrature: Simpson, Trapezoidal methods
Numerical integration of initial value problems, Runge Kutta method
Shooting methods

7. Multiple ODE's (3)
   Simplest method: solving reaction network problems with multiple reactions
   Connections to multiple algebraic equations (eigenvalues etc.)

8. PDE's (3)
   Parabolic PDE's (heat conduction problem)
   Other boundary conditions

9. Optimization (3)

As time permits, one or more of the following topics: Monte Carlo integration, molecular dynamics as an example of second order ODE's, stability and chaos

ChE 253K (Introduction to Statistics and Data Analysis)

1. Introduction (2)
   Discrete vs. continuous
   Variance of measurements
   Value of statistical analysis

2. Descriptive Statistics (3)
   Data sorting
   Frequency tables
   Stem and leaf plots
   Histograms
   Pareto plots
   Ogive plots

3. Probability (2)
   Defining probability
   Counting techniques, permutation and combination
   Additivity and Multiplicative rules
   Bayes' rule

4. Working with discrete random variables and probability distributions (2)
   Define discrete random variables and continuous variables
   Binomial distribution
   Hypergeometric distribution
   Poisson distribution

5. Working with Continuous Probability Distributions (2)
   Normal distribution
   Normal approximation to the binomial

Chi-Squared distribution

6. Functions of Random Variables (1)
   - Moments and moment generating functions

7. One and two Sample Estimations (3)
   - Statistical inference
   - Estimating the mean
   - Standard error
   - Tolerance limits
   - Estimating the difference between two means
   - Paired observations
   - Estimating variance
   - Estimating the ratio of variances

8. Hypothesis Testing (3)
   - Concepts
   - One and two tailed tests
   - Use of p-values
   - Choice of sample size
   - Tests of means
   - Tests of Variance

9. Linear Regression and Correlation (4)
   - Least square estimators
   - Analysis of variance approach
   - Linear regression case studies

10. Second Factorial Experiments (3)
    - Concepts of statistical experimental design and response surface analysis
    - Introduction to JMP for Box Behnken, etc.
    - Design of experiments and Response surface analysis with JMP

11. Statistical Process Control (2)
    - Nature of control limits
    - Purposes of control charts
    - X-bar charts
    - R-bar charts
    - Cusum control charts