

Ben-Gurion University

Most students find it difficult to learn programming and in practice very few of them do any programming after finishing the basic course on the subject. After over 35 years that programming has been taught in the Chemical Engineering Departments, many schools now consider dropping those studies altogether because of their ineffectiveness.

At the Ben-Gurion University we have removed the required programming course from the curriculum two years ago and at the same time we extended an existing “Introduction to Personal Computers (IPC)” course by incorporating MATLAB programming into it. The main objective of the IPC course is to enable the students to solve engineering problems that involve complex consecutive calculations, solving linear and nonlinear algebraic and ordinary differential equations, and carrying out multiple linear and polynomial regression, using POLYMATH, Excel and MATLAB. To enhance the learning effectiveness the following advanced features are included in the course:

Based on real life problems – the study of each subject starts by presenting a real life problem, which requires numerical solution using one of the techniques mentioned above. Typical benchmark problems used include the calculation of thermodynamic properties using a cubic equation of state (Shacham et al, 2003), calculation of flow rate in draining a tank (Brauner and Shacham, 1994), calculation of adiabatic flame temperature (Shacham, 1998) and correlation of vapor pressure data using the Clapeyron, Antoine and Riedel’s equations (Shacham et al, 1996).

Multi-stage problems – the problems require computer solution in several stages. Preliminary stages are solvable with the “user friendly” software packages (POLYMATH, Excel) while advanced stages require MATLAB programming (Shacham et al, 2003).

Programming by modification – solved examples are provided. The students are encouraged to modify and extend the solved examples to solve their assignments.

Self-grading – students check and grade their own homework assignments and exams. The self-test program provides feedback on the errors made (Shacham, 1998). Most students will not be satisfied unless they get a working program that yields correct results.

The problem-based approach ensures that the students understand the need in learning programming and this increases their motivation. Using *multi-state problems* and *programming by modification* ensures that the students can get a working program in a reasonable length of time without losing faith in their programming abilities. The *self-grading* aspect provides an additional incentive to get a working program that yields correct results.

The final exam of the course in this last semester included the use of the “secant” method for solution of the adiabatic flame temperature problem (Shacham, 1998) with MATLAB programming. The students had an hour and a half to complete this assignment and 75% of them (40 students) managed to get a working program that yielded the correct solution. This clearly demonstrates the effectiveness of the teaching techniques that have been used in the IPC course.

Introduction to Modeling and Computation for Chemical Engineers with POLYMATH, Excel and MATLAB

Chapter 1: Complex Consecutive Calculations (pdf file, 233 KB)

Homework assignment **1:** Calculation of Molar Volume and Compressibility

Factor of a Gas Using the Redlich – Kwong Equation of State.

- a. Problem Definition
- b. Self Test

Chapter 2: Iterative Solution of a Nonlinear Equation (pdf file, 256 KB)

Homework assignment **2:** Calculation of Adiabatic Flame Temperature

- a. Problem Definition
- b. Self Test

Homework assignment **3:** Calculation of Molar Volume and Compressibility

Factor Using Various Equations of State.

- a. Problem Definition
- b. Self Test

Homework assignment **4:** Bubble Point and Dew Point for an Ideal Multi-component Mixture

- a. Problem Definition
- b. Self Test

Chapter 3: Matrix Operations and Solution of Systems of Linear Equations (pdf file, 193 KB)

Chapter 4: Multiple-Linear, Polynomial and Nonlinear Regression. Part I (pdf file, 215 KB), Part II (pdf file, 310 KB)

Homework assignment **5:** Fitting Correlations (Regression Models) to Vapor Pressure Data

- a. Problem Definition
- b. Self Test

Homework assignment **6:** Linearization of the Antoine Equation

- a. Problem Definition
- b. Self Test

Chapter 5. Introduction to Solution of Systems of Nonlinear Algebraic Equations

Chapter 6. Introduction to solution of Systems of Ordinary Differential Equations (pdf file, 263 KB)

Comments, Corrections and Suggestions

Comments, corrections and suggestions regarding this course are welcome and should be sent to: shacham@bgumail.bgu.ac.il

References (Section B.2)

Brauner, N. and M. Shacham, "Numerical Experiments in Fluid Mechanics with a Tank and Draining Pipe", *Comput. Appl. Eng. Educ.*, **2**(3), 175-183 (1994).

Shacham, M., N. Brauner and M.B. Cutlip, "Replacing the Graph Paper by Interactive Software in Modeling and Analysis of Experimental Data", *Comput. Appl. Eng. Educ.*, **4**(3), 241-251 (1996).

Shacham, M., "Computer Based Exams in Undergraduate Engineering Courses", *Comput. Appl. Eng. Educ.*, **6**(3) 3, 210-209 (1998).

Shacham, M., N. Brauner and M.B. Cutlip, "An Exercise for Practicing Programming in the ChE Curriculum", *Chem. Eng. Educ.*, **37**(2), 148 (2003).