Integration of Numerical Problem Solving into the Chemical Engineering Curriculum

Michael B. Cutlip and Mordechai Shacham

Department of Chemical Engineering, University of Connectcut, Unit 3222, Storrs, CT 06269-3222 /
Department of Chemical Engineering, Ben-Gurion University of the Negev. Beer Sheva, Israel 84105

ABSTRACT

This paper provides a collection of representative problems with detailed solutions that can be used to introduce numerical problem solving into core chemical engineering courses. These problems require application of the numerical analysis areas of linear equations, nonlinear equations, ordinary differential equations, partial differential equations, and regressions with statistics (polynomial, multiple linear and nonlinear).

A set of 12 "example" problems is presented along with complete solutions utilizing three representative software packages: Microsoft Excel*, MATLAB*, and Polymath*. An additional set of 12 "assignment" problems is also be presented. All 24 problem statements and detailed solutions are made available on a special web site that has been designed for efficient use by interested faculty.

These problems and their solutions provide insight into the various types of problems appropriate to chemical engineering, practical aspects of problem solution, and proper interpretations of results. Emphasis will be given to placement of these problems and application of the software within the Chemical Engineering curriculum.

INTRODUCTION

Engineering computations often require the use numerical software packages for problem solving. Such needs frequently arise in both ChE education and practice, where the main objectives are deriving the mathematical model of the physical phenomena and critically analyzing the results while technical details of the solution can be handled by a numerical software package. For professionals and ChE students who are involved with the development of mathematical models, there are considerable benefits in using numerical software packages for model development and implementation as compared to the use of source code programming. This is particularly helpful when engineers must carry out computations that involve non-conventional processes and chemi-

* Excel is a trademark of Microsoft Corporation (http://www.microsoft.com), MATLAB is a trademark of The Math Works, Inc. (http://www.mathworks.com), and POLYMATH is copyrighted by Mordechai Shacham, Michael B. Cutlip, and Michael Elly (http://www.polymath-software.com).

cals. Such processes cannot be modeled with the standard flow sheeting programs, and the use of numerical software packages in such cases is usually most effective.
These problems and their supporting materials were originally created and collected for a workshop the ASEE Chemical Engineering Division Summer School held at the University of Colorado in Boulder from July 27 to August 1, 2002. The materials are intended to provide a resources for faculty members who desire to introduce numerical calculations within their engineering courses. The problem statements and detailed solution can be used or easily modified for course use. The mathematical packages utilized in this work are widely available, and most students can have easy access to the software package on their own personal computers.

PROBLEMS

Two collections of representative problems are available. The first set was used in the workshop in which many of the details were discussed and demonstrations of the solutions were given. A summary of these "demonstration" problems is given in Table 1. Here the appropriate courses where these problems can be introduced are suggested. Note that the mathematical models required in the problems encompass most of the standard numerical analysis topics that undergraduates typically study in their coursework.

Table 1 Set of Demonstration Problems Illustrating the Use of Numerical Methods[a]

COURSE	PROBLEM DESCRIPTION	MATHEMATICAL MODEL	DEMO PROBLEM
Introduction to Ch. E.	Steady State Material Balances on a Separation Train	Simultaneous Linear Equations	D1
Introduction to Ch. E.& Thermodynamics	Molar Volume and Compressibility Factor from Van Der Waals Equation	Single Nonlinear Equation	D2
Thermodynamics & Separation Processes	Three Phase Equilibrium - Bubble Point	Simultaneous Nonlinear Equations	D3
Fluid Dynamics	Terminal Velocity of Falling Particles	Single Nonlinear Equation	D4
Thermodynamics & Reaction Engineering	Reaction Equilibrium for Multiple Gas Phase Reactions	Simultaneous Nonlinear Equations	D5
Mathematical Methods	Vapor Pressure Data Representation by Polynomials and Equations	Polynomial Fitting, Linear and Nonlinear Regression	D6
Heat Transfer	Unsteady State Heat Exchange in a Series of Agitated Tanks	Simultaneous ODE's with Known Initial Conditions	D7
Mass Transfer & Reaction Engineering	Diffusion with Chemical Reaction in a One Dimensional Slab	Simultaneous ODE's with Split Boundary Conditions	D8
Reaction Engineering	Reversible, Exothermic, Gas Phase Reaction in a Catalytic Reactor	Simultaneous ODE's and Explicit Algebraic Equations	D9

Table 1 Set of Demonstration Problems Illustrating the Use of Numerical Methods[a]

COURSE	PROBLEM DESCRIPTION	MATHEMATICAL MODEL	DEMO PROBLEM
Process Dynamics and Control	Dynamics of a Heated Tank with PI Temperature Control	Simultaneous Stiff ODE's	D10
Separation Processes	Binary Batch Distillation	Simultaneous ODE's and Nonlinear Algebraic Equations (Differential Algebraic Equations)	D11
Heat Transfer	Unsteady-state Heat Conduction in a Slab	Partial Differential Equation	D12

[a]These problems are taken in part from "Problem Solving in Chemical Engineering with Numerical Methods" by Michael B. Cutlip and Mordechai Shacham, Prentice-Hall (1999).

An addition set of problems referred to as the "assignment" problems set that was intended for a "hands-on" computing laboratory at the Summer School is summarized in Table 2. The combined problem sets in Tables 1 and 2 and their detailed solutions with Excel, MATLAB, and Polymath provide a very substantial base of numerical problems for faculty use.

Table 2 Set of Assignment Problems Illustrating the Use of Numerical Methods[a]

COURSE	PROBLEM DESCRIPTION	MATHEMATICAL MODEL	ASSIGNMENT PROBLEM
Introduction to Ch. E.	Steady State Material Balances on a Separation Train*	Simultaneous Linear Equations	A1
Introduction to Ch. E.& Thermodynamics	Molar Volume and Compressibility Factor from Redlich-Kwong Equation	Single Nonlinear Equation	A2
Thermodynamics & Separation Processes	Dew Point and Two-Phase Flash in a Non-Ideal System	Simultaneous Nonlinear Equations	A3
Fluid Dynamics	Pipe and Pump Network	Simultaneous Nonlinear Equations	A4
Reaction Engineering	Operation of a Cooled Exothermic CSTR	Simultaneous Nonlinear Equations	A5
Mathematical Methods	Vapor Pressure Correlations for a Sulfur Compound Present in Petroleum	Polynomial Fitting, Linear and Nonlinear Regression	A6
Reaction Engineering	Catalyst Decay in a Packed Bed Reactor Modeled by a Series of CSTRs	Simultaneous ODE's with Known Initial Conditions	A7
Mass Transfer	Slow Sublimation of a Solid Sphere	Simultaneous ODE's with Split Boundary Conditions	A8
Reaction Engineering	Semibatch Reactor with Reversible Liquid Phase Reaction	Simultaneous ODE's and Explicit Algebraic Equations	A9

Table 2 Set of Assignment Problems Illustrating the Use of Numerical Methods[a]

COURSE	PROBLEM DESCRIPTION	MATHEMATICAL MODEL	ASSIGN-MENT PROBLEM
Process Dynamics and Control	Reset Windup in a Stirred Tank Heater	Simultaneous ODE's with Step Functions	A10
Reaction Engineering & Process Dynamics and Control	Steam Heating Stage of a Batch Reactor Operation	Simultaneous ODE's and Explicit Algebraic Equations	A11
Mass Transfer & Mathematical Methods	Unsteady State Mass Transfer in a Slab	Partial Differential Equation	A12

[a]These problems are taken in part from "Problem Solving in Chemical Engineering with Numerical Methods" by Michael B. Cutlip and Mordechai Shacham, Prentice-Hall (1999).

INTERNET WEB SITE

A special web site has been created to provide the problem details and the additional resources that can be helpful in their solutions. This web site is:

http://www.engr.uconn.edu/~cutlipm/ASEE2003/

The web site is organized as is shown in the following screen display: The types of files are indicated.

Application of Mathematical Software Packages in Chemical Engineering Education
ASEE Annual Meeting 2003 - Paper from Session 2797
Michael B. Cutlip and Mordechai Shacham

General Introduction DOC PDF HTM

A. General Materials
  Demonstration Problems PDF
  Assignment Problems PDF
B. POLYMATH
  POLYMATH Solutions to Demonstration Problems PDF
    POLYMATH Solution Files DIR
    POLYMATH Introduction DOC PDF HTM
    POLYMATH Detailed Overview DOC PDF HTM
C. MATLAB
  MATLAB Presentation PPT PDF
  MATLAB Solution Files XLS
  MATLAB Regression Files XLS
D. EXCEL
  EXCEL Presentation PPT PDF
  EXCEL Solution Files XLS
E. Software Installation Files
  POLYMATH Demo Instructions DOC PDF HTM
  POLYMATH Demo Software (limited to 20 sessions) SETUP
  Request Full Examination Copy of POLYMATH Software DOC PDF HTM

The General Introduction provide an overview and the objectives of the presented materials. The General Materials section provides detailed problem statements of the 24 problems that comprise the demonstration and assignment problem sets. Each presented problem a specific indication of the Numerical Methods, the Concepts Utilized, the Course Usage, and the Problem Statement.

Introductory materials for each of the mathematical packages are given along with the actual solutions. Solutions files are also provided. An examination copy of POLYMATH is available for download to allow the use of this software. An inexpensive site license is available for POLYMATH from the CACHE Corporation (http://www.cache.org). MATLAB is generally available to academics, and examination copies are available from the Mathworks web site (http://www.mathworks.com). EXCEL is usually available to faculty and students as a part of the Microsoft Office suite of software. Most computer laboratories have several of these packages available for general use.

CONCLUDING REMARKS

The problems presented on the web site and their details solutions with three different mathematical software packages should allow interested faculty to introduce numerical problem solving into many courses within Chemical Engineering and related engineering disciplines. Judicious use of these and similar problems can assist in the integration of numerical problem solving into the curriculum. Such introduction is educationally appropriate, interesting to students, and relatively easily achieved by faculty. Numerical problem solving allows for the solution of realistic engineering problems, and the gradual introduction of numerical problems into core courses is well-received by students. Such usage encourages the appropriate use of numerical methods for problem solving on the student's own personal computer and thus becomes a very useful education tool. Many departments choose to provide a numerical analysis course at some point in the curriculum for those students who wish to have more knowledge of the numerical methods used in these software packages. These problems are also useful in this type of course.

BIOGRAPHICAL INFORMATION

Michael B. Cutlip is professor of chemical engineering at the University of Connecticut in Storrs, CT where he has been on the faculty for 35 years. He is co-author of POLYMATH, a numerical analysis package, which is widely used by chemical engineering students. He has been particularly active with the AICHE and the ASEE Chemical Engineering Division having served as Division Programming Chair for the Seattle Annual Meeting in 1998 and was the Division Chair in 2000. He was also a co-chair of the ASEE Chemical Engineering Division Summer School in 2002 at the University of Colorado.

Mordechai Shacham is a Professor in the Department of Chemical Engineering at the Ben Gurion University of the Negev in Beer-Sheva, Israel where he has served as Department Head. He is the principal author of POLYMATH, a numerical analysis package, which is widely used in chemical engineering throughout the world. Professor Shacham is co-author of the Prentice Hall textbook "Problem Solving in Chemical Engineering with Numerical Methods." He is a past president of the Israel Institute of Chemical Engineers, and he is an active member of the Chemical Engineering Division of ASEE.