Historical Perspective on Numerical Problem Solving

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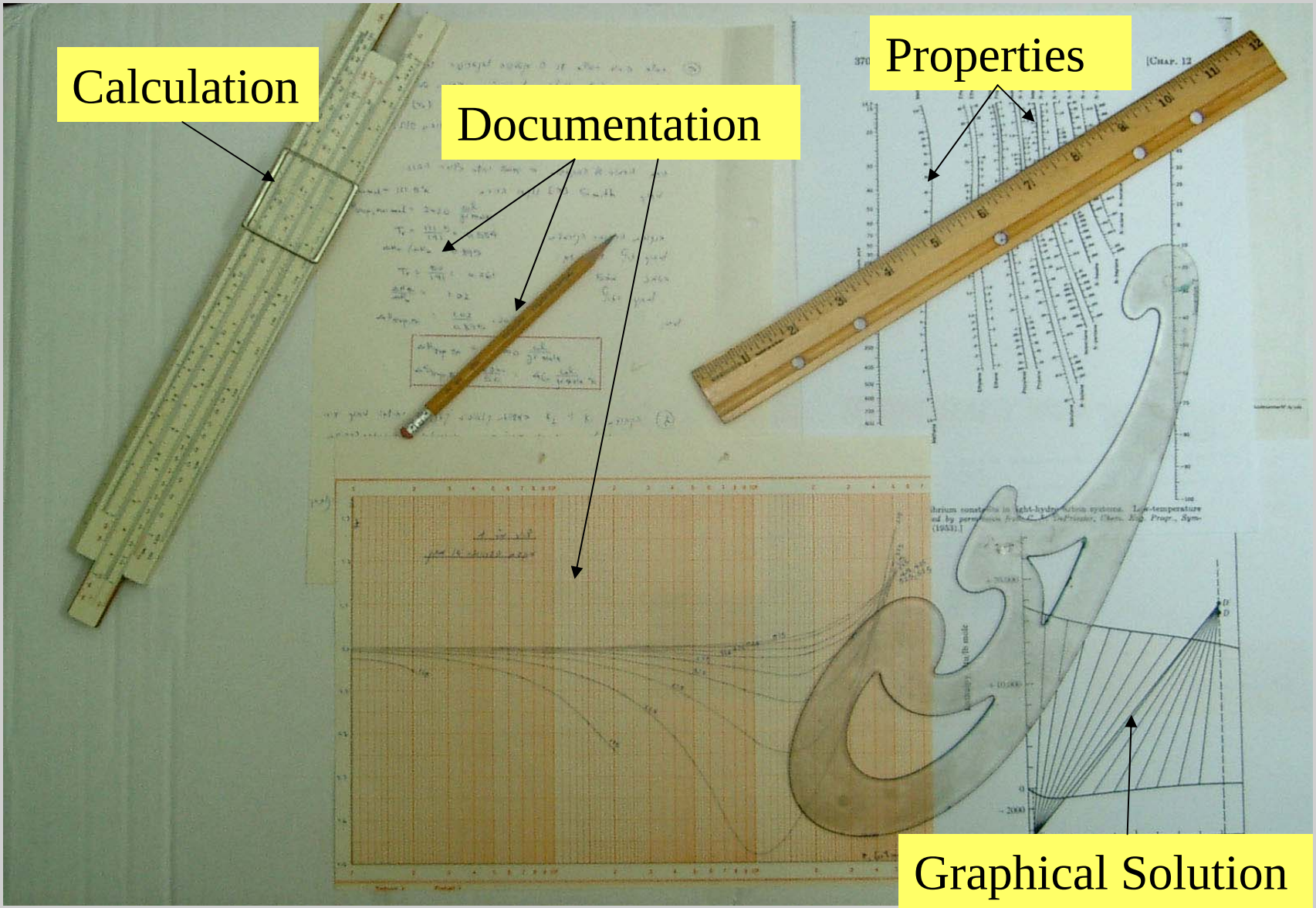
Typical Chemical Engineering Problems for Numerical Solution

COURSE	PROBLEM TITLE	MATHEMATICAL MODEL	PROBLEM
Introduction to Ch. E.	Molar Volume and Compressibility Factor from Van Der Waals Equation	Single Nonlinear Equation	1
Introduction to Ch. E.	Steady State Material Balances on a Separation Train*	Simultaneous Linear Equations	2
Mathematical Methods	Vapor Pressure Data Representation by Polynomials and Equations	Polynomial Fitting, Linear and Nonlinear Regression	3
Thermodynamics	Reaction Equilibrium for Multiple Gas Phase Reactions*	Simultaneous Nonlinear Equations	4
Fluid Dynamics	Terminal Velocity of Falling Particles	Single Nonlinear Equation	5
Heat Transfer	Unsteady State Heat Exchange in a Series of Agitated Tanks*	Simultaneous ODE's with known initial conditions.	6
Mass Transfer	Diffusion with Chemical Reaction in a One Dimensional Slab	Simultaneous ODE's with split boundary conditions.	7
Separation Processes	Binary Batch Distillation**	Simultaneous Differential and Nonlinear Algebraic Equations	8
Reaction Engineering	Reversible, Exothermic, Gas Phase Reaction in a Catalytic Reactor*	Simultaneous ODE's and Algebraic Equations	9
Process Dynamics and Control	Dynamics of a Heated Tank with PI Temperature Control**	Simultaneous Stiff ODE's	10

Chemical Engineer's Tools of Trade - 1965



Chemical Engineer's Problem Solution Techniques - 1965

Analytical solutions, including

- Model simplification by neglecting less important terms
- Model manipulation to bring it into a solvable form

Short-cut solution techniques

- Replacing the problem with a simpler one that can be solved

Graphical solutions

Trial and error solution techniques

Numerical solution, including

- Computer language programming and debugging

Shortcomings of the Traditional Solution Techniques

Manual and Graphical Solution Techniques

Tedious, time consuming error prone process

Oversimplification may lead to wrong results

Highest precision is two decimal digits

Time constraints prevent screening of large number of alternatives to find an optimal solution

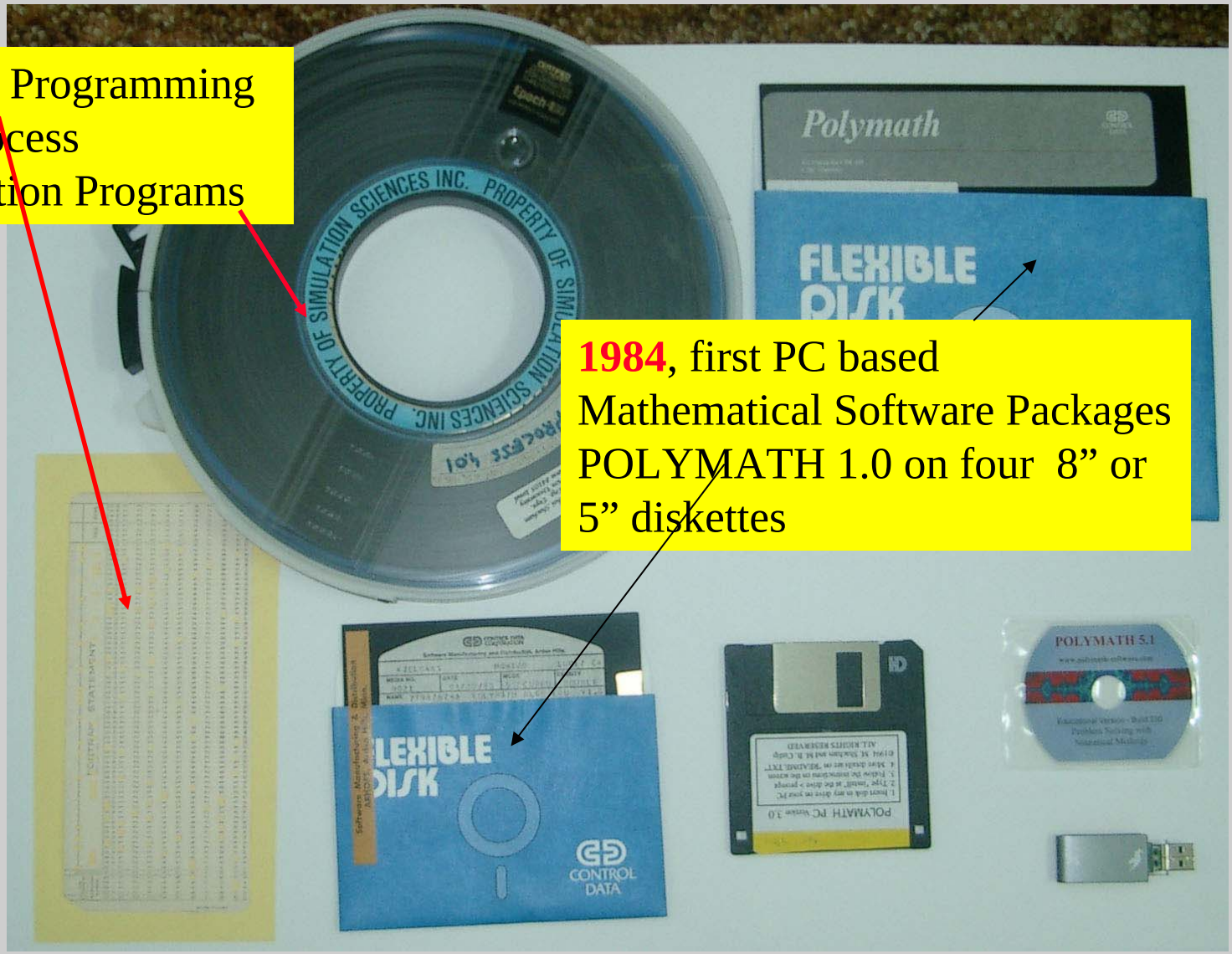
Computer Language Programming

Requires experts in programming, numerical and optimization methods

Tedious, time consuming error prone process

First Milestones of Computer Use for Problem Solving

Fortran Programming and Process Simulation Programs



1984, first PC based Mathematical Software Packages POLYMATH 1.0 on four 8” or 5” diskettes

A Typical Fortran Program (Circa 1969*)

```
C       .....PRINT VARIOUS RESULTS, AS APPROPRIATE .....
        WRITE (6,206) ITER, TAG1, TAG2
        WRITE (6,207)
        DO 4 I = 1, N
    4   WRITE (6,205) (ANEW(I,J), J = 1, N)
        IF (EIGVEC) GO TO 5
           WRITE (6,208)
           GO TO 1
    5   IF (.NOT. TAG1) GO TO 6
           WRITE (6,209)
           GO TO 1
    6   IF (.NOT. TAG2) GO TO 7
           WRITE (6,210)
           GO TO 1
    7   WRITE (6,211)
        DO 8  I = 1, N
    8   WRITE (6,205) (U(I,J), J = 1, N)
        GO TO 1
C
C       ..... FORMATS FOR INPUT AND OUTPUT STATEMENTS .....
  100   FORMAT (6X, E7.1, 10X, E7.1, 10X, E7.1, 10X, F4.1/
     1 6X, I3, 11X, L2)
  101   FORMAT (3X, I3, 11X, I4, 2(12X, L2))
  102   FORMAT (10X, 14F5.1)
```

*Carnahan,Luther and Wilkes, *Applied Numerical Methods*, Wiley

- Non-intuitive commands and syntax rules make the program difficult and time consuming to prepare and debug.
- Only large and complex assignments worth the effort of computer solution.

Milestones in the Use of Mathematical Software Packages (MSP)in Problem Solving (Personal View)

1984 - Publication of the PC based Mathematical Software Packages

1992 – Publication of a CRE Textbook where an MSP is Integrated into the Solution Process

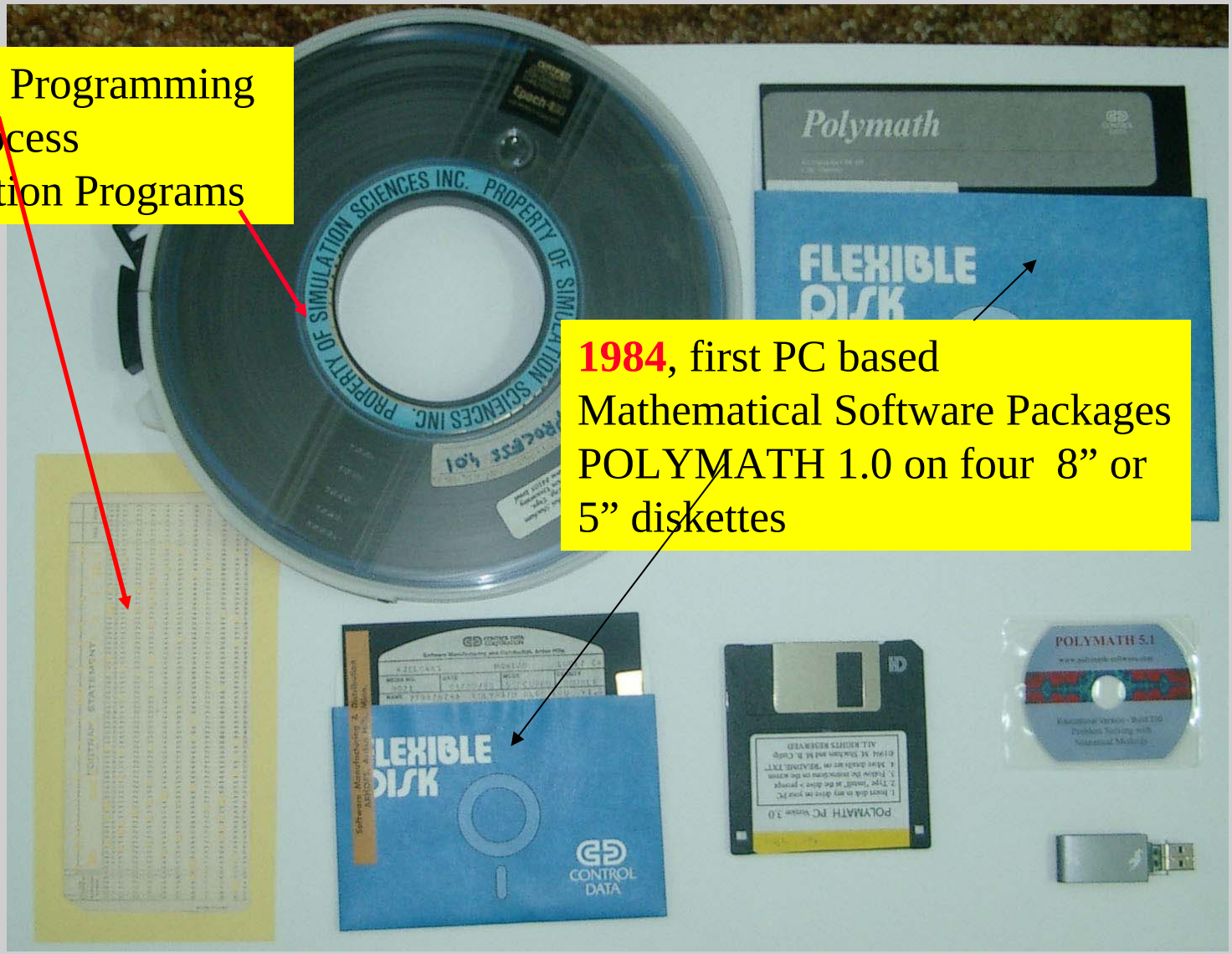
1997 – ASEE Summer School – A Set of 10 Representative ChE Problems are Solved Using Excel, Polymath, MATLAB, Mathcad, Mathematica, Maple

2002 – ASEE Summer School - Manual Conversion of the POLYMATH Model to Excel and MATLAB is Advocated for Efficient Problem Solving

2007 – ASEE Summer School - Automatic Conversion of the POLYMATH Model to Excel and MATLAB for Parametric Studies and Solution of Multiple Model and/or Multiple Algorithmic Probs.

First Milestones of Computer Use for Problem Solving

Fortran Programming and Process Simulation Programs



1984, first PC based Mathematical Software Packages POLYMATH 1.0 on four 8” or 5” diskettes

How Should POLYMATH be Used in CRE courses?

Fogler H. S., "An Appetizing Structure of Chemical Reaction Engineering for Undergraduates", *Chem. Eng. Ed.*, **27**(2), 110(1993)

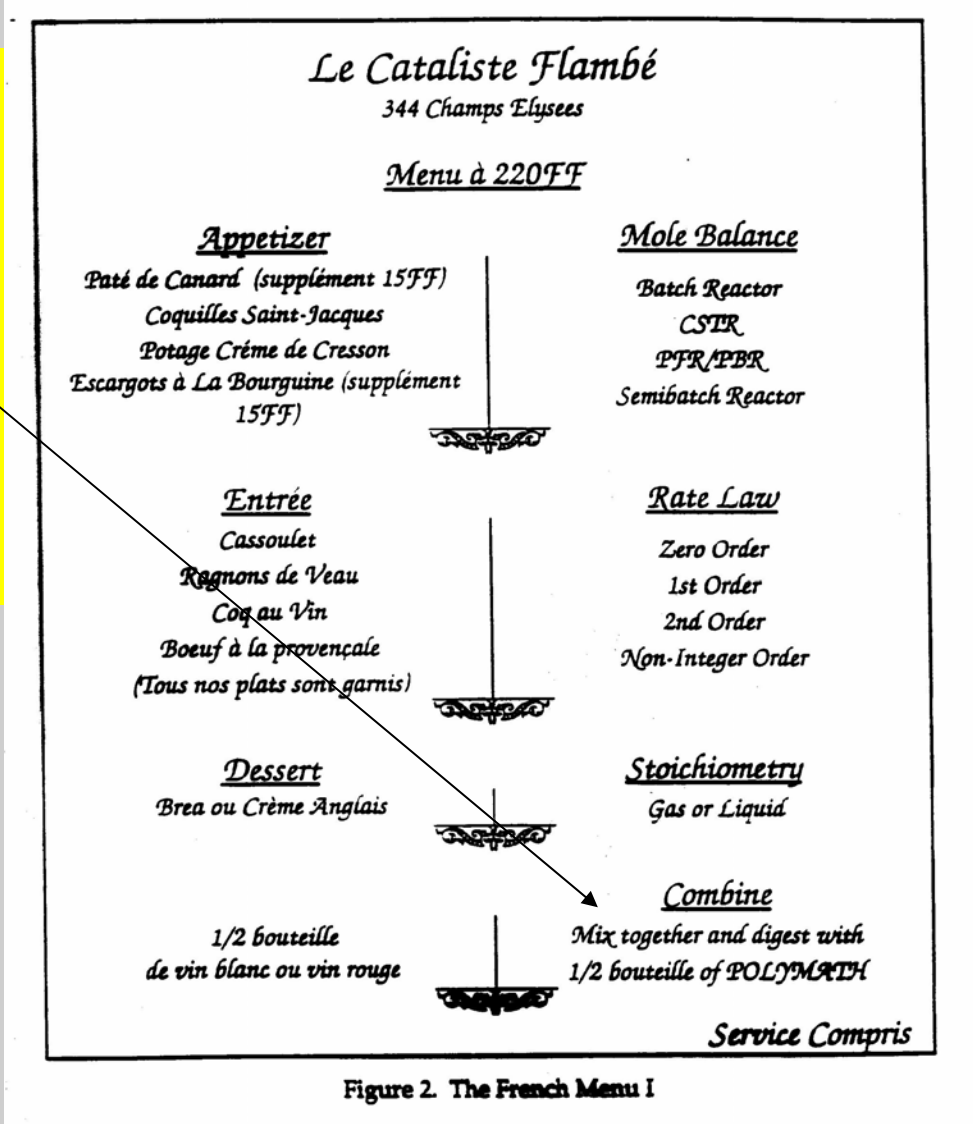


Figure 2. The French Menu I

ASEE Chemical Engineering Summer School Snowbird, Utah, 1997, Problems

COURSE	PROBLEM TITLE	MATHEMATICAL MODEL	PROBLEM
Introduction to Ch. E.	Molar Volume and Compressibility Factor from Van Der Waals Equation	Single Nonlinear Equation	1
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Problem Statements and Solutions are available at

http://www.polymath-software.com/ASEE/index.htm

ASEE Chemical Engineering Summer School Snowbird, Utah, 1997, Solutions

The particular individual who has considerable experience with a particular mathematical package is responsible for the solution with that package

- Excel - Edward M. Rosen, EMR Technology Group
- Maple - Ross Taylor, Clarkson University
- Mathematica - H. Eric Nuttall, University of New Mexico
- Mathcad - John J. Hwalek, University of Maine
- MATLAB - Joseph Brule, John Widmann, Tae Han, and Bruce Finlayson, Department of Chemical Engineering, University of Washington
- POLYMATH - Michael B. Cutlip, University of Connecticut and Mordechai Shacham, Ben-Gurion University of the Negev

This selection of problems should help chemical engineering faculty evaluate which mathematical problem solving package they wish to use in their courses and should provide some typical problems in various courses which can be utilized.

Problem Statements and Solutions are available at

http://www.polymath-software.com/ASEE/index.htm

ASEE Chemical Engineering Summer School Snowbird, Utah, 1997, Conclusions*

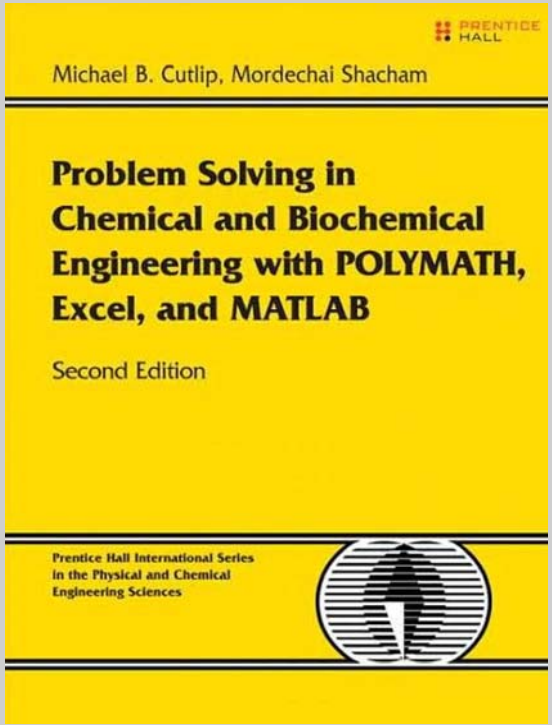
All of the mathematical software packages were able to correctly solve the ten benchmark problems, but there were considerable differences in the "user friendliness" and the technical effort required to set up the model and document the model and the solution.

Our work and experience with mathematical software has lead us to conclude that the most educational benefit can be gained by using several packages throughout the curriculum.

This is the same conclusion reached by Jones ("The Non-Use of Computers in Undergraduate Engineering Science Courses", *J. Engr. Ed*., **87**(1), 11 ,1998) . after he conducted a computer use survey.

*Shacham, M. and M.B. Cutlip, “A Comparison of Six Numerical Software Packages for Educational Use in the Chemical Engineering Curriculum”, *Computers in Education Journal*, IX(3), 9-15 (1999)

ASEE Chemical Engineering Summer School Pullman, WA, 1997



Chapters

1. **Introduction***
2. Basic Principles and Calculations
3. Regression and Correlation of Data
4. **Problem Solving with Excel***
5. **Problem Solving with MATLAB***
6. Advanced Techniques in Problem Solving.
7. Thermodynamics
8. Fluid Mechanics
9. Heat transfer
10. Mass Transfer
11. Chemical Reaction Engineering
12. Phase Equilibria and Distillation
13. Process Dynamics and Control
14. Biochemical Engineering

*Partially Covered in the Summer School Workshop

ASEE Chemical Engineering Summer School Pullman, WA, 2007

Book Usage in Various Courses

An introductory course of Computer Based Problem Solving (CBPS)

1. Introduction
2. Basic Principles and Calculations
3. Regression and Correlation of Data
4. Problem Solving with Excel
5. Problem Solving with MATLAB
6. Advanced Techniques in Problem Solving.
7. Thermodynamics

Examples for Numerical Methods and Advanced Math Courses

8. Fluid Mechanics
9. Heat transfer
10. Mass Transfer
11. Chemical Reaction Engineering
12. Phase Equilibria and Distillation
13. Process Dynamics and Control
14. Biochemical Engineering

Categorizing Problems According to the Solution Technique Used

Basic Topics

(a) Consecutive Calculations
(b) System of Linear Algebraic Equations
(c) One Nonlinear (Implicit) Algebraic Equation
(d) Multiple Linear and Polynomial Regressions
(e) Systems of First-Order Ordinary Differential Equations (ODE's) - Initial Value problems
(f) System of Nonlinear Algebraic Equations (NLE)

Advanced Topics

(g) Higher Order ODE's
(h) Systems of First-Order ODEs - Boundary Value Problems
(i) Stiff Systems of First-Order ODE's
(j) Differential-Algebraic System of Equations (DAE's)
(k) Partial Differential Equations (PDE)
(l) Nonlinear Regression
(m) Parameter Estimation in Dynamic Systems
(n) Nonlinear Programming (Optimization) with Equity Constraints

Session Outline

	Subject	Duration
Introduction	Historical Perspective on Numerical Problem Solving	20 min
Example 1	Molar Volume and Compressibility Factor from Redlich-Kwong Equation Sequential Calculations with POLYMATH and Excel, Parm. Studies with Excel	20 min
Example 2	Calculation of the Flow Rate in A Pipeline Solution of a Single Nonlinear (Implicit) Algebraic Equation with POLYMATH and MATLAB, Parametric Studies with MATLAB	20 min
Example 3	Multiple Linear, Polynomial and Nonlinear Regression with Statistical Analysis	25 min
Example 4	Adiabatic Operation of a Tubular Reactor for Cracking of Acetone Solution of a System of ODEs with POLYMATH and Excel, Parametric Studies with Excel	15 min
Example 5	Complex Chemical Equilibrium Solution of a System of Nonlinear Algebraic Equations (NLE) with POLYMATH and MATLAB, Parametric Studies with MATLAB	15 min
Example 6	Simultaneous Multi-component Diffusion of Gases Solution of a System of ODEs with POLYMATH and MATLAB, Boundary Value Iterations with MATLAB	15 min
MiscProbs	Brief Review of Problem Types not Discussed in Detail: Stiff ODEs, DAEs, PDEs, parameter estimation, nonlinear programming, multiple model – multiple algorithm problems	15 min
Conclusions	Conclusions and Discussion	5 min