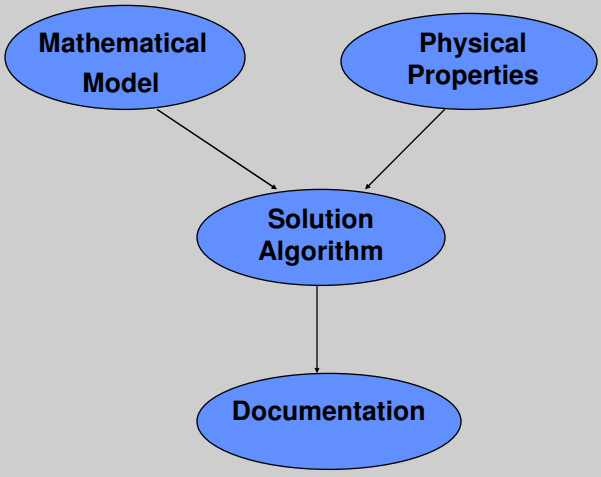
Modern Problem Solving Techniques in Engineering with POLYMATH, Excel and MATLAB.

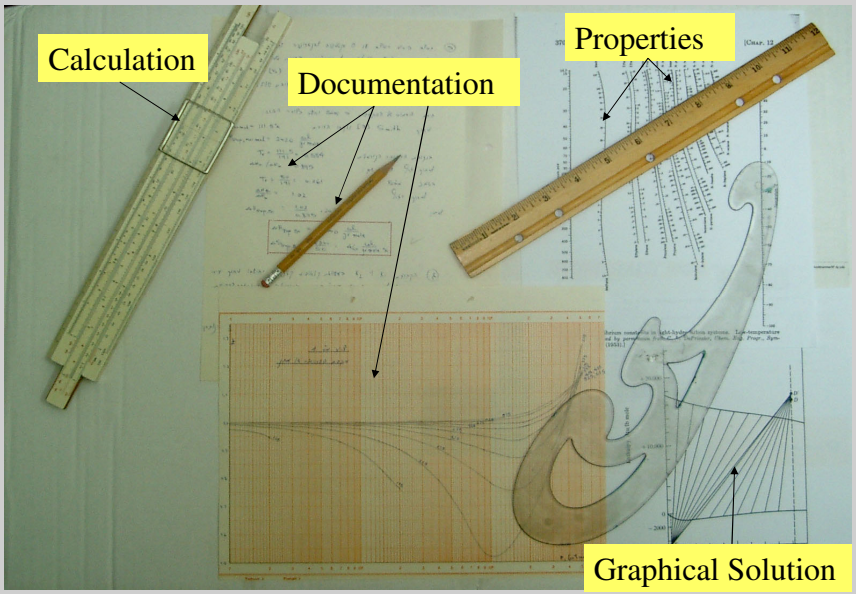
Introduction

Engineers are fundamentally problem solvers, seeking to achieve some objective or design among technical, social economic, regulatory and environmental constraints

Problem Solving in Chemical Engineering



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

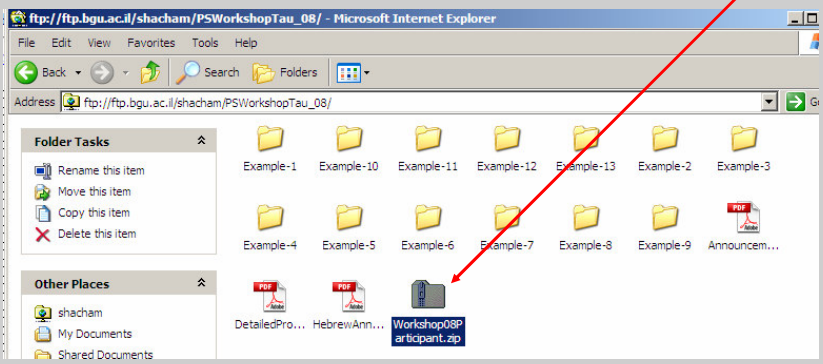
Requires experts in programming, numerical and optimization methods

Tedious, time consuming error prone process

First Milestones of Computer Use for Problem Solving

Workshop Material Availability

All the workshop material is available on the ftp site:
ftp://ftp.bgu.ac.il/shacham/PSWorkshopTau_08/
The complete set of the workshop notes, presentations, Polymath, Excel and MATLAB files can be downloaded as one zip file: Workshop08Participant.zip or individual files and folders can be downloaded separately.



Sequential Calculations with POLYMATH and Excel, Parametric Studies with Excel

A typical example is the solution of cubic equations of state for the compressibility factor for specified value of the temperature T and pressure P.

$$R = 0.08206$$
$$T_c = 304.2$$
$$P_c = 72.9$$
$$b = RT_c/(8P_c)$$
$$a = (27/64)(R^2T_c^{\,2}/P_c)$$
$$P = R\cdot T/(V-b) - a/V^2$$

Solution is easily obtained by Polymath for a few sets of values of T and P. Excel or MATLAB are needed to carry out the calculations for large sets of data

Sequential Calculations with POLYMATH and Excel, Parametric Studies with Excel

Example 1
Molar Volume and Compressibility Factor from Redlich-Kwong Equation

Example-1.pdf	Presentation Handouts
Prob_4.1.pdf	Example problem in the book of Cutlip and Shacham
Example1_A.pol	Polymath solution file
Example1_B1.xls	Excel solution, compressibility factor
Example1_B1.xls	Excel solution, molar volume

Solution of a Single Nonlinear (Implicit) Algebraic Equation with POLYMATH and MATLAB, Parametric Studies with MATLAB

A single nonlinear equation can be written in the form

$$f(x) = 0$$

where f is a function and x is the unknown. Additional explicit equations may also be included.

Typical examples belonging to this category include:

- ❖Solving various equations of state for molar volume and/or compressibility factor
- ❖Bubble point, dew point and isothermal flash calculations for ideal multi-component mixtures
- ❖Calculation of adiabatic flame temperature in combustion.
- ❖ Calculation of the flow rate in a pipeline.

Multiple Linear and Polynomial Regression with Statistical Analysis

Given a set of data of measured (or observed) values of a dependent variable: y_i versus n independent variables x_{1i}, x_{2i}, … x_{ni}, multiple linear regression attempts to find the "best" values of the parameters a_0, a_1, …a_n for the equation

$$\hat{y}_i = a_0 + a_1 x_{1,i} + a_2 x_{2,i} + \ldots + a_n x_{n,i}$$

$\hat{y}_i$ is the calculated value of the dependent variable at point i. The "best" parameters have values that minimize the squares of the errors

$$S = \sum_{i=1}^{N} (y_i - \hat{y}_i)^2$$

In polynomial regression there is only one independent variable, thus

$$\hat{y}_i = a_0 + a_1 x_i + a_2 x_i^2 + \ldots + a_n x_i^n$$

Multiple Linear Regression with Statistical Analysis

Correlation of Heat of Hardening of Portland Cement versus Composition

Example-3.pdf	Presentation Handouts
Example_3.pol	Polymath data file
RegrOverview.pdf	Equations, Statistics, Graphs and Examples

Polynomial and Nonlinear Regression with Statistical Analysis

Correlating Temperature Dependent Physical Properties

Example-4.pdf	Presentation Handouts
Prob_4.4.pdf	Example problem in the book of Cutlip and Shacham
CpEthane.pol	Polymath data file (Heat capacity)
VpEthane.pol	Polymath data file (Vapor pressure)
WagnerEq.pol	Polymath solution file (Wagner equation)

Topic 5	Solution of a System of ODEs with POLYMATH and Excel, Parametric Studies with Excel
Example 5	Adiabatic Operation of a Tubular Reactor for Cracking of Acetone
Topic 6	Solution of a System of Nonlinear Algebraic Equations (NLE) with POLYMATH and MATLAB, Parametric Studies with MATLAB
Example 6	Complex Chemical Equilibrium
Topic 7	Solution of Multiple-Model, Multiple-Algorithm Problems
Example 7	Semi-continuous Fed-Batch and Cyclic- Fed Batch Operation of a Bioreactor
Topic 8	Estimating Model Parameters for Dynamic Models
Example 8	Modeling Reproduction Rate of a Microorganism in a Fermenter
Topic 9	Constrained Minimization with POLYMATH and Excel
Example 9	Complex Chemical Equilibrium by Gibbs Energy Minimization

Topic 10	Solution of a System of ODEs with POLYMATH and MATLAB, Boundary Value Iterations with MATLAB
Example 10	Simultaneous Multicomponent Diffusion of Gases
Topic 11	Method of Lines for Partial Differential Equations
Example 11	Diffusion and Reaction in a Falling Laminar Liquid Film
Topic 12	Applications in Environmental Engineering
Example 12	Numerical Simulations with the Oxygen-sag model
Topic 13	Applications in Process Safety
Example 13	HAZOP Analysis of a Process for Oxidation of 2-octanol in a semi-batch reactor

Practical Use of the Material Studied in the Workshop

Educational version of the Polymath 6.1 program, for personal use of the Workshop participants is available at http://www.polymath-software.com/trial. The following user name and password should enable you to enter the site:

User Name: *psworkshop*

Password: *tau2008*

Download the file: *PolymathEduTrial261.exe*, save it on your computer and run it in order to install Polymath 6.1

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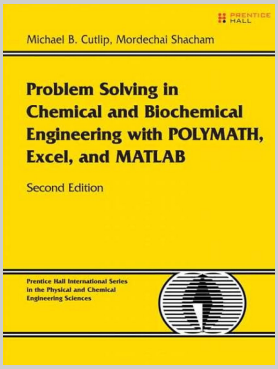

Chapters

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

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

Examples for Numerical Methods and Advanced Math Courses

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

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