The PEM System for Chemical Engineering Problem Solving – Five Examples

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PEM - Increases Problem Solving Efficiency and Capabilities with a Novel Combination of Software Tools

• Polymath© (easy problem formulation)
• Excel™ (familiar spreadsheet environment)
• MATLAB™ (advanced problem solving)

Students and professionals at their personal computers or in computer labs can now effectively solve problems using all the above packages.
PEM Desktop Problem Solving Involving Polymath, Excel, and MATLAB

- Mathematical Model
  - Polymath 6.1
    - Solution Algorithm
      - Excel Solution
        - Excel
        - Polymath Solution
          - MATLAB
            - MATLAB Solution
POLYMATH Educational (EDU) or POLYMATH Professional (PRO)

• Extremely Easy-to-Use
• Excellent Problem Solving Capabilities
  – Linear Equations – 100 (264 PRO)
  – Nonlinear Equations – 30 (300 PRO)
  – Differential Equations – 30 (300 PRO)
  – Regressions (Linear, Polynomial, Multiple Linear, Nonlinear) - 301 data points (1001 PRO)
• Automated Export of Problems to Working Excel Spreadsheets Enabling Stand-Alone Excel Calculations (Provides Add-In for Excel that Solves ODEs). (EDU and PRO)
• Enables the Use MATLAB by Automatically Translating Problems to Code for Use in M-files. (EDU and PRO)
POLYMATH 6.1 features include:

• EASE OF USE WITHOUT ANY PROGRAMMING LANGUAGES OR CONTROL LANGUAGES TO REMEMBER
• STANDARD WINDOWS EDITING
• EXTENSIVE USER ALGORITHM SELECTION AND CONTROL
• EXECUTION WITH ALL 32-BIT WINDOWS OPERATING SYSTEMS INCLUDING VISTA
• COMPATIBILITY WITH PREVIOUS VERSIONS
• THREE ON-BOARD UTILITIES: POWERFUL CALCULATOR, UNIT CONVERTER, AND EXTENSIVE ENGINEERING CONVERSION FACTORS
• EXTENSIVE ON-LINE DOCUMENTATION
• AUTOMATIC PROBLEM EXPORT TO EXCEL – EXCEL ADD-IN FOR DIFFERENTIAL EQUATIONS
• MATLAB OUTPUT GIVING ORDERED AND FORMATTED EQUATIONS
Polymath Software has Four Main Programs

- LEQ Linear Equations
- NLE Nonlinear Equations
- DEQ Differential Equations
- REG Regression
Polymath Software also has Three Utilities:

- Calculator
- Units Converter
- Scientific Constants
Initial Polymath Software Display with Help that Gives Detailed Information on the Software
Extensive On-Line HELP

Welcome to POLYMATH 6.X

Polymath has four major programs:

Please open Polymath and Review the On-Line Help!
Five Sample Problems

1. Linear Equations – Material Balances for Distillation Columns – Polymath
2. Explicit Calculations – Equation of State – Polymath and Excel
5. Regressions – Vapor Pressure Data (Linear and Nonlinear) - Polymath, Excel
Working the Sample Problems

You will be able to work with the five sample problems if you have access to POLYMATH, Excel and MATLAB on your personal computer.

POLYMATH Educational (for students and faculty) or POLYMATH Professional can be downloaded for 15-days of free use from

[POLYMATH Educational 15-day Trial](#)

[POLYMATH Professional 15-day Trial](#)

It is recommended that you download and install POLYMATH Software and the ODE_Solver Add-In in preparation for solving the example problems. Also you should install Excel and MATLAB if possible.

Clicking on the green boxes with the file names below in the following pages will automatically load the files directly into the appropriate program. You should try to keep this presentation in one window and work on the problem in another window while keeping both visible. This will be very convenient for working the sample problems.

Please close the programs and related windows when each sample problem is completed.
Workshop Problem 1

Numerical Solution: Linear Equations

Title: Material Balances for a Train of Distillation Columns

Software Used: Polymath
Problem 1 – Linear Equations for Material Balances for a Train of Distillation Columns

Determine Molar Flow Rates $B_1$, $D_1$, $B_2$, and $D_2$
Problem 1 – Linear Equations for Material Balances for a Train of Distillation Columns

Select a part of the flow sheet for making balances as show in red.
Problem 1 – Linear Equations for Material Balances for a Train of Distillation Columns

Make Balances on Each Species:
Xylene
Styrene
Toluene
Benzene

Determine Flow Rates B1, D1, B2, and D2

Xylene: $0.07D_1 + 0.18B_1 + 0.15D_2 + 0.24B_2 = 0.15 \times 70$
Styrene: $0.04D_1 + 0.24B_1 + 0.10D_2 + 0.65B_2 = 0.25 \times 70$
Toluene: $0.54D_1 + 0.42B_1 + 0.54D_2 + 0.10B_2 = 0.40 \times 70$
Benzene: $0.35D_1 + 0.16B_1 + 0.21D_2 + 0.01B_2 = 0.20 \times 70$
Problem 1 – Linear Equations for Material Balances for a Train of Distillation Columns

Xylene: $0.07D_1 + 0.18B_1 + 0.15D_2 + 0.24B_2 = 10.5$
Styrene: $0.04D_1 + 0.24B_1 + 0.10D_2 + 0.65B_2 = 17.5$
Toluene: $0.54D_1 + 0.42B_1 + 0.54D_2 + 0.10B_2 = 28$
Benzene: $0.35D_1 + 0.16B_1 + 0.21D_2 + 0.01B_2 = 14$

Polymath Program Exercise

Use Polymath to Enter and Solve Equations

OR

Click Here to Use Polymath Solution File to Solve Equations

Select Program LEQ – Linear Equations, Change Number of Equations to 4 and Press Enter. Then Enter Problem Data.

LinearEquations01.pol
Workshop Problem 2

Numerical Solution: Explicit Equations

Title: Explicit Calculations for an Equation of State

Software Used: Polymath and Excel
Problem 2 - Explicit Calculations for an Equation of State

Calculate $P$ when the other variables and parameters of the van der Waals equation of state are known.

$$R = 0.08206$$

$$T_c = 304.2$$

$$P_c = 72.9$$

$$T = 350$$

$$V = 0.6$$

$$a = \frac{24}{64}((R^2T_c^2)/P_c)$$

$$b = \frac{RT_c}{8P_c}$$

$$P = \frac{RT}{(V - b) - a/V^2}$$

Hint: Use POLYMATH Nonlinear Equations Solver (even when there are no nonlinear equations).
Problem 2 - Explicit Calculations for an Equation of State
Polymath Solution Demonstration

Enter the equations into Polymath.

Note that the equations can be entered in any order. Polymath orders equations before solution.

Use templates or full screen editor.
Problem 2 - Explicit Calculations for an Equation of State

Polymath Solution Exercise

Click here to import this problem solution into POLYMATH and solve problem to verify given solution.

PolymathNonlinear.pol

NonlinearEquations01.pol

R = 0.08206
Tc=304.2
Pc=72.9
T=350
V=0.6
a=(24/64)*((R^2*Tc^2)/Pc)
b=(R*Tc)/(8*Pc)
P=(R*T)/(V-b)-a/V^2
Problem 2 - Explicit Calculations for an Equation of State
Polymath Solution then Export to Excel for Solution
Problem 2 - Explicit Calculations for an Equation of State

Polymath Solution then Export to Excel for Solution Exercise

Hint – Be sure to have an open EXCEL Spreadsheet running on your computer before exporting problem.

Export the POLYMATH problem to EXCEL by clicking the EXCEL icon.

\[
\begin{align*}
R &= 0.08206 \\
Tc &= 304.2 \\
Pc &= 72.9 \\
T &= 350 \\
V &= 0.6 \\
a &= \frac{(24/64)((R^2*Tc^2)/Pc)} \\
b &= \frac{(R*Tc)}{(8*Pc)} \\
P &= \frac{(R*T)}{(V-b)-a/V^2}
\end{align*}
\]
Problem 2 - Explicit Calculations for an Equation of State

Polymath Solution then Export to Excel for Solution Exercise

<table>
<thead>
<tr>
<th></th>
<th>A</th>
<th>B</th>
<th>C</th>
<th>D</th>
<th>E</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>POLYMATH NLE Migration Document</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>Explicit Eqs</td>
<td>Variable</td>
<td>Value</td>
<td>Polymath Equation</td>
<td></td>
</tr>
<tr>
<td>3</td>
<td></td>
<td>R</td>
<td>0.08206</td>
<td>R=0.08206</td>
<td></td>
</tr>
<tr>
<td>4</td>
<td></td>
<td>Tc</td>
<td>304.2</td>
<td>Tc=304.2</td>
<td></td>
</tr>
<tr>
<td>5</td>
<td></td>
<td>Pc</td>
<td>72.9</td>
<td>Pc=72.9</td>
<td></td>
</tr>
<tr>
<td>6</td>
<td></td>
<td>T</td>
<td>350</td>
<td>T=350</td>
<td></td>
</tr>
<tr>
<td>7</td>
<td></td>
<td>V</td>
<td>0.6</td>
<td>V=0.6</td>
<td></td>
</tr>
<tr>
<td>8</td>
<td></td>
<td>a</td>
<td>3.20542178</td>
<td>a=(24/64)<em>((R^2</em>Tc^2)/Pc)</td>
<td></td>
</tr>
<tr>
<td>9</td>
<td></td>
<td>b</td>
<td>0.0428029</td>
<td>b=(R<em>Tc)/(8</em>Pc)</td>
<td></td>
</tr>
<tr>
<td>10</td>
<td></td>
<td>P</td>
<td>42.6415451</td>
<td>P=(R*T)/(V-b)-a/V^2</td>
<td></td>
</tr>
</tbody>
</table>

Compare your EXCEL results to the POLYMATH results.
Workshop Problem 3

Numerical Solution: Nonlinear Equations

Title: Pressure Drop Calculations for Pipe Flow

Software Used: Polymath and Excel
Problem 3 – Nonlinear Equations - Pressure Drop Calculations for Pipe Flow

Polymath Solution for Two Nonlinear Equations – Simultaneous Solution with If… Then… Else… Statement

Pressure Drop Equation

\[ dp = 2 \times fF \times \rho \times v \times v \times L / D \]

becomes in Polymath

\[ f(D) = dp - 2 \times fF \times \rho \times v \times v \times L / D \]

The nonlinear equation is always rearranged to equal zero.
Friction Factor Equation

\[ f_F = \frac{16}{Re} \quad \text{if} \quad Re < 2100 \]

\[ = \frac{1}{4 \log(Re \sqrt{f_F}) - 0.4}^2 \quad \text{if} \quad Re \geq 2100 \]

becomes in Polymath

\[ f(f_F) = \textbf{If} \ (Re < 2100) \textbf{Then} (f_F - \frac{16}{Re}) \]
\[ \textbf{Else} (f_F - \frac{1}{(4 \log(Re \sqrt{f_F}) - 0.4)^2}) \]

The second nonlinear equation uses the If… Then… Else… Statement
Problem 3 – Nonlinear Equations - Pressure Drop Calculations for Pipe Flow

Polymath Solution for Two Nonlinear Equations – Simultaneous Solution with If… Then… Else… Statement

Solution will be made in Polymath and Excel
Problem 3 – Nonlinear Equations - Pressure Drop Calculations for Pipe Flow

POLYMATH Demonstration - Two Nonlinear Equations – Simultaneous Solution with If… Then… Else… Statement

This is an example of two nonlinear equations plus nine explicit equations.

# Calculation of pipe diameter to have Pressure Drop of 103000 Pa over Length of 100 meters.
f(D) = dp - 2 * fF * rho * v * L / D # Calculation of pipe diameter for specified flowrate (D in m)
f(fF) = If (Re < 2100) Then (fF - 16 / Re) Else (fF - 1 / (4 * log(Re * sqrt(fF)) - 0.4) ^ 2) # Fanning's friction factor

# The explicit equations
rho = 46.048 + T * (9.418 + T * (-0.0329 + T * (4.882e-5 - T * 2.895e-8))) # Liquid density (kg/cu-m)
vis = exp(-10.547 + 541.69 / (T - 144.53)) # Liquid viscosity (Pa-s)
Re = D * v * rho / vis # Reynold's number
v = q / (pi * D ^ 2 / 4) # Flow velocity (m/s)
dp = 103000 # Pressure drop (Pa)
L = 100 # Pipe length (m)
T = 25 + 273.15 # Temperature (K)
pi = 3.1416
q = 0.0025 # Flow rate (cu-m/s)

# Initial Guess for nonlinear equations variables
D(0) = 0.04
fF(0) = 0.004
Problem 3 – Nonlinear Equations - Pressure Drop Calculations for Pipe Flow

POLYMATH Demonstration - Two Nonlinear Equations – Simultaneous Solution with If... Then... Else... Statement

The nonlinear equations for pressure drop and for Fanning friction factor will be solved to be zero.

The nonlinear equations for pressure drop and for Fanning friction factor will be solved to be zero.
Problem 3 – Nonlinear Equations - Pressure Drop
Calculations for Pipe Flow

POLYMATH Demonstration - Two Nonlinear Equations –
Simultaneous Solution with If... Then... Else... Statement

Here is the Polymath solution

### Calculated values of NLE variables

<table>
<thead>
<tr>
<th>Variable</th>
<th>Value</th>
<th>f(x)</th>
<th>Initial Guess</th>
</tr>
</thead>
<tbody>
<tr>
<td>D</td>
<td>0.0389653</td>
<td>4.133E-09</td>
<td>0.04</td>
</tr>
<tr>
<td>ff</td>
<td>0.0045905</td>
<td>-8.674E-19</td>
<td>0.004</td>
</tr>
</tbody>
</table>

### Variable Value

<table>
<thead>
<tr>
<th>Variable</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>dp</td>
<td>1.03E+05</td>
</tr>
<tr>
<td>L</td>
<td>100.</td>
</tr>
<tr>
<td>pi</td>
<td>3.1416</td>
</tr>
<tr>
<td>q</td>
<td>0.0025</td>
</tr>
<tr>
<td>Re</td>
<td>9.097E+04</td>
</tr>
<tr>
<td>rho</td>
<td>994.5715</td>
</tr>
<tr>
<td>T</td>
<td>298.15</td>
</tr>
<tr>
<td>v</td>
<td>2.096491</td>
</tr>
<tr>
<td>vis</td>
<td>0.0008931</td>
</tr>
</tbody>
</table>

### Nonlinear equations

1. \( f(D) = \frac{\Delta p}{2} \cdot 2 \cdot f_F \cdot \rho \cdot \frac{v}{L} \cdot \frac{D}{D} = 0 \)
   - Calculation of pipe diameter for specified flowrate \(D\) in m

2. \( f(f_F) = \begin{cases} \text{If } (\text{Re} < 2100) & \text{Then } \frac{f_F}{16} \cdot \text{Re} \text{ Else } \frac{f_F}{1} \cdot \left(4 \cdot \log(\text{Re}) - 0.4\right)^2 = 0 \end{cases} \)
   - Fanning's friction factor

### Explicit equations

1. \( T = 25 + 273.15 \)
   - Temperature (K)

2. \( \rho = 45.048 + T \cdot (9.418 + T \cdot (-0.0329 + T \cdot (4.882 \cdot 5 - T \cdot 2.895 \cdot 8))) \)
   - Liquid density (kg/cu-m)

3. \( \pi = 3.1416 \)

4. \( q = 0.0025 \)
   - Flow rate (cu-m/s)

5. \( \Delta p = 103000 \)
   - Pressure drop (Pa)

6. \( L = 100 \)
   - Pipe length (m)

7. \( \text{vis} = \exp(-10.547 + 541.69 / (T - 144.53)) \)
   - Liquid viscosity (Pa-s)

8. \( v = \frac{q}{(\pi \cdot D^2 / 4)} \)
   - Flow velocity (m/s)

9. \( \text{Re} = \frac{D \cdot v \cdot \rho}{\text{vis}} \)
   - Reynold's number
Problem 3 – Nonlinear Equations - Pressure Drop Calculations for Pipe Flow

POLYMATH/Excel Demonstration - Two Nonlinear Equations – Simultaneous Solution with If… Then… Else… Statement

Polymath Software has the option of automatically sending a problem to Excel where the problem is ready to be solved. For Nonlinear Equations, you will use the Solver Add-In to obtain Excel solution.

# Calculation of pipe diameter to have Pressure Drop of 103000 Pa over Length
f(D) = dp - 2 * fF * rho * v * v * L / D # Calculation of pipe diameter for specified
f(fF) = If (Re < 2100) Then (fF - 16 / Re) Else (fF - 1 / (4 * log(Re * sqrt(fF))))
Problem 3 – Nonlinear Equations - Pressure Drop Calculations for Pipe Flow

POLYMATH/Excel Demonstration - Two Nonlinear Equations – Simultaneous Solution with If... Then... Else... Statement

From Polymath

To Excel

One Key Press automatically creates problem in Excel.

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**POLYMATH NLE Migration Document**

<table>
<thead>
<tr>
<th>A</th>
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<th>C</th>
<th>D</th>
<th>E</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Variable</td>
<td>Value</td>
<td>Polymath Equation</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>rho</td>
<td>994.5715</td>
<td>rho=46.048 + T * (9.418 + T * (-0.0329 + T * (4.8 + T / 100)))</td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>vis</td>
<td>0.0008931</td>
<td>vis=exp(-10.547 + 541.69 / (T - 144.53))</td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>Re</td>
<td>88620.363</td>
<td>Re=D * v * rho / vis</td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>v</td>
<td>1.9894321</td>
<td>v=q / (pi * D ^ 2 / 4)</td>
<td></td>
</tr>
<tr>
<td>6</td>
<td>dp</td>
<td>103000</td>
<td>dp=103000</td>
<td></td>
</tr>
<tr>
<td>7</td>
<td>L</td>
<td>100</td>
<td>L=100</td>
<td></td>
</tr>
<tr>
<td>8</td>
<td>T</td>
<td>298.15</td>
<td>T=25 + 273.15</td>
<td></td>
</tr>
<tr>
<td>9</td>
<td>pi</td>
<td>3.1416</td>
<td>pi=3.1416</td>
<td></td>
</tr>
<tr>
<td>10</td>
<td>q</td>
<td>0.0025</td>
<td>q=0.0025</td>
<td></td>
</tr>
<tr>
<td>11</td>
<td>D</td>
<td>0.04</td>
<td>D(0)=0.04</td>
<td></td>
</tr>
<tr>
<td>12</td>
<td>fF</td>
<td>0.004</td>
<td>fF(0)=0.004</td>
<td></td>
</tr>
<tr>
<td>13</td>
<td>f(D)</td>
<td>24272.898</td>
<td>f(D)=dp - 2 * fF * rho * v * v * L / D</td>
<td></td>
</tr>
<tr>
<td>14</td>
<td>f(f(F))</td>
<td>-0.000695</td>
<td>f(f(F))=f(f(F))</td>
<td></td>
</tr>
<tr>
<td>15</td>
<td>Sum of Squares:</td>
<td>589173571</td>
<td>F = f(f(F))^2 + f(f(F))^2</td>
<td></td>
</tr>
</tbody>
</table>
Problem 3 – Nonlinear Equations - Pressure Drop Calculations for Pipe Flow Excel Demonstration

Use Excel Add-In Solver For Solution

Excel Solution
Problem 3 – Nonlinear Equations - Pressure Drop Calculations for Pipe Flow - Excel EXCERCISE

1) Obtain the Polymath Solution

Click here for Polymath Problem Solution File
NonlinearEquations02.pol

2) Export the Problem to Excel by Clicking on Excel Icon

First Open Excel (click here) before Export and Have Solver Add-In Available for Use in Solution
Excel.xls

3) Solve the Same Problem in Excel

Or Click here for Excel Solution File
NonlinearEquations02.xls
Workshop Problem 4

Numerical Solution: Simultaneous Ordinary Differential Equations

Title: Batch Reactor

Software Used: Polymath, Excel and MATLAB
Consider a Batch Reactor that initially has only reactant A at a value of 1. The reactions are first order and irreversible. Reaction time t is from 0 to 3.

\[
\begin{align*}
A & \xrightarrow{k_1} B \xrightarrow{k_2} C \\
\text{l. C. for } t = 0, \ t_{\text{final}} = 3
\end{align*}
\]

\[
\begin{align*}
\frac{dC_A}{dt} &= -k_1 C_A & \text{l. C. } C_A|_{t=0} = 1 \\
\frac{dC_B}{dt} &= k_1 C_A - k_2 C_B & \text{l. C. } C_B|_{t=0} = 0 \\
\frac{dC_C}{dt} &= k_2 C_B & \text{l. C. } C_C|_{t=0} = 0 \\
k_1 &= 2 & k_2 &= 3
\end{align*}
\]
Problem 4 - Differential Equations - Batch Reactor

Differential Equations – Simultaneous ODEs

POLYMATH/Excel Solution EXERCISE

Click Here to Enter and Solve this Problem in POLYMATH
PolymathDifferential.pol
Or Open Polymath

Click Here to Use Problem Solution in POLYMATH
DifferentialEquations01.pol
Problem 4 - Differential Equations - Batch Reactor
POLYMATH/Excel Solution EXERCISE

1) Open Excel, 2) Export Polymath Problem to Excel, and 3) Solve with Polymath ODE_Solver Add-In.

Click here to Open Excel
Excel.xls  or Open Excel

Click here to Open Problem, Export and Solve in Excel
DifferentialEquations01.pol

OR

Click here for Excel Solution File
DifferentialEquation01.xls
Problem 4 - Differential Equations - Batch Reactor
POLYMATH/MATLAB Solution Demonstration

Let’s Look at the MATLAB Solution
MATLAB problem solution is obtained by first requesting MATLAB output in the Polymath Setting window found with the Settings Icon.
This option for MATLAB formatted output results in the MATLAB code to be generated automatically at the end of the POLYMATH report.

**Matlab Formatted Problem Code**

tspan = [0 4.]; % Range for the independent variable
y0 = [1.; 0; 0]; % Initial values for the dependent variables
function dYfuncvecdt = ODEfun(t,Yfuncvec);
CA = Yfuncvec(1);
CB = Yfuncvec(2);
CC = Yfuncvec(3);
k1 = 2;
k2 = 3;
dCAdt = 0 - (k1 * CA);
dCBdt = k1 * CA - (k2 * CB);
dCCdt = k2 * CB;
dYfuncvecdt = [dCAdt; dCBdt; dCCdt];
Problem 4 - Differential Equations - Batch Reactor

POLYMATH/MATLAB Solution Demonstration

The MATLAB formatted output is copied and pasted into the MATLAB template that is provided within the Polymath HELP materials.

3. Differential Equations

The MATLAB program template for a Polymath program involving differential equations is given in the box below. This can be copied into the MATLAB editor and saved as MultipleDEQtemplate.m for future use.

```matlab
function % Insert here your file name after function (Use Alphanumeric names only)
clear, clc, format short g, format compact
tspan= % Replace this line with tspan line from Polymath report
y0= % Replace this line with y0 line from Polymath report
disp(' Variable values at the initial point ');
disp([t = num2str(tspan(1))]);
disp(' y dy/dt ');
disp([y0 ODEfun(tspan(1),y0)]);
[t,y]=ode45(@(ODEfun,tspan,y0);
for i=1:size(y,2)
disp([' Solution for dependent variable y'' int2str(i)]);
disp([' t y'' int2str(i)]);
disp([t y(:,i)]);
plot(t,y(:,i));
title([' Plot of dependent variable y'' int2str(i)]);
xlabel(' Independent variable (t)');
ylabel([' Dependent variable y'' int2str(i)];
pause
end
%-----------------------------
% Replace this and the following line with the function copied from the Polymath report
% Do not include the tspan and y0 lines
```
Problem 4 - Differential Equations - Batch Reactor

MATLAB Code from Polymath is Entered into Template. Yellow bars indicate copied code.

```matlab
function MATLAB01
    clear, clc, format short g, format compact
    ts vão [0 4]; \% Range for the independent variable
    y0 = [1; 0; 0]; \% Initial values for the dependent variables
    disp(' Variable values at the initial point ');
    disp([' t = ' num2str(tspan(1))]);
    disp([' y dy/dt ']);
    disp([y0 ODEfun(tspan(1),y0)]);
    [t,y]=ode45(@ODEfun,tspan,y0);
    for i=1:size(y,2)
        disp([' Solution for dependent variable y' int2str(i)]);
        disp([' t y(:,i)]);
        plot(t,y(:,i));
        title([' Plot of dependent variable y' int2str(i)]);
        xlabel(' Independent variable (t)');
        ylabel([' Dependent variable y' int2str(i)]);
        pause
    end
    \%----------------------------------------
    function dYfuncvecdt = ODEfun(\tau,Yfuncvec);
    CA = Yfuncvec(1);
    CB = Yfuncvec(2);
    CC = Yfuncvec(3);
    k1 = 2;
    k2 = 3;
    dCADt = 0 - (k1 * CA);
    dCBdt = k1 * CA - (k2 * CB);
    dCCdt = k2 * CB;
    dYfuncvecdt = [dCADt; dCBdt; dCCdt];
```
The MATLAB m-file thus created provides graphical output for all differential variables.
Problem 4 - Differential Equations - Batch Reactor

The MATLAB m-file thus created provides graphical output for all differential variables.

MATLAB Solution Demonstration
Problem 4 - Differential Equations - Batch Reactor

The MATLAB m-file thus created provides graphical output for all differential variables.

MATLAB Solution Demonstration
Problem 4 - Differential Equations - Batch Reactor
MATLAB Solution Demonstration

The MATLAB m-file thus created also provides tabular output within the MATLAB editor.
Problem 4 - Differential Equations - Batch Reactor
POLYMATH/MATLAB Solution EXERCISE

1) Obtain the Polymath Solution with options to generate MATLAB Code

Click here for Polymath Solution File
DifferentialEquations01.pol

2) Start MATLAB, Open MATLAB Template for Multiple Differential Equations, Enter MATLAB Code from Polymath, and Solve Problem.

Click here for MATLAB files that need to be placed in your working MATLAB directory. For MATLAB, a right mouse click should be used to 'Save Target As..' to indicate the location of your desired working directory for MATLAB.

MultipleDEQtemplate.m MATLAB01.m
Workshop Problem 5

Numerical Solution: Linear and Nonlinear Regression

Title: Vapor Pressure Data

Software Used: Polymath and Excel
The Clapeyron equation is commonly used to correlate vapor pressure \((P_v)\) with absolute temperature \((T)\) in °C where \(\Delta H_v\) is the latent heat of vaporization and \(R\) is the gas constant. This equation can be written with two parameters, \(D\) and \(E\), when \(\Delta H_v\) is constant with temperature. \(P_v\) is typically in mm Hg and \(T\) is usually in °C.

\[
\log P_v = -\frac{\Delta H_v}{RT} + B = \frac{D}{T} + E
\]

Another common vapor pressure correlation is the Antoine equation, which utilizes three parameters given by \(A\), \(B\), and \(C\).

\[
\log P_v = A + \frac{B}{T + C}
\]

Determine the values of \(D\) and \(E\) for the Clapeyron equation and the values of \(A\), \(B\), and \(C\) for the Antoine equation using the data given below. Compare these correlations.

Vapor Pressure Data

<table>
<thead>
<tr>
<th>(T) (°C)</th>
<th>41.77</th>
<th>56.69</th>
<th>69.66</th>
<th>84.78</th>
<th>95.65</th>
<th>100.18</th>
<th>114.79</th>
<th>123.40</th>
</tr>
</thead>
<tbody>
<tr>
<td>(P) (mm Hg)</td>
<td>100</td>
<td>200</td>
<td>300</td>
<td>500</td>
<td>700</td>
<td>900</td>
<td>1200</td>
<td>1500</td>
</tr>
</tbody>
</table>
Problem 5 – Regressions - Vapor Pressure Data

Regressions – Linear and Nonlinear

Mathematical Model

Polymath 6.1

Solution Algorithm

Excel Solution

Excel

Polymath Solution
Problem 5 – Regressions - Vapor Pressure Data

POLYMATH Clapeyron Equation Linear Regression EXERCISE

Utilize the Polymath Regression Program to input the data to the Data Table.

Create a new column for a variable \( \log P \) that is the log of the pressure.

\[ \log P = \log(P) \]

Then create another column for a variable \( \text{invT} \) that is the inverse of the temperature in \( ^\circ \text{C} \).

\[ \text{invT} = \frac{1}{T} \]
Problem 5 – Regressions - Vapor Pressure Data

Utilize the Polymath Regression Program to make a Linear Regression of logP versus invTK to yield the parameters D and E of the Clapeyron equation.

\[
E = a_0 = 3.658 \\
D = a_1 = -73.61
\]

Click here for Polymath Problem Data File

OR

Click here for Polymath Solution File

Polymath Data File is RegressionData01.pol
Polymath Solution File is Regression01.pol
Problem 5 – Regressions - Vapor Pressure Data

POLYMATH/Excel Solution EXERCISE

The Graph Option from the Polymath Regression Program indicates a reasonable representation of the data.

However, the Residuals Plot Option shows a trend in the errors.
Problem 5 – Regressions - Vapor Pressure Data

POLYMATH/Excel Solution EXERCISE

Utilize the Export to EXCEL Option from the Polymath Regression Program to make a Linear Regression of logP versus invTK. The results, shown below, are essentially the same as those obtained with Polymath.

<table>
<thead>
<tr>
<th>A</th>
<th>B</th>
<th>C</th>
<th>D</th>
<th>E</th>
<th>F</th>
<th>G</th>
<th>H</th>
<th>I</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>POLYMATH Polynomial Regression Migration Document</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>invT</td>
<td>logP</td>
<td>logP calc</td>
<td>logP residual</td>
<td>logP residual ^2</td>
<td>a1</td>
<td>a0</td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>0.0239406</td>
<td>2</td>
<td>1.895103293</td>
<td>-0.104896707</td>
<td>0.011003319</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>0.0176399</td>
<td>2.30103</td>
<td>2.358946908</td>
<td>0.057916908</td>
<td>0.003354368</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>6</td>
<td>0.0143554</td>
<td>2.477121</td>
<td>2.600733343</td>
<td>0.123612343</td>
<td>0.015280011</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>7</td>
<td>0.0117952</td>
<td>2.69897</td>
<td>2.789206619</td>
<td>0.090236619</td>
<td>0.008142647</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>8</td>
<td>0.0104548</td>
<td>2.845098</td>
<td>2.88788234</td>
<td>0.04278434</td>
<td>0.0018305</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>9</td>
<td>0.009982</td>
<td>2.954243</td>
<td>2.922688279</td>
<td>-0.031554721</td>
<td>0.0009957</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>10</td>
<td>0.0087116</td>
<td>3.079181</td>
<td>3.016210836</td>
<td>-0.062970164</td>
<td>0.003965242</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>11</td>
<td>0.0081037</td>
<td>3.176091</td>
<td>3.060962381</td>
<td>-0.115128619</td>
<td>0.013254599</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Click here for EXCEL Problem Solution File (for those who need it)

File is Regression01.xls
Utilize the Polymath Regression Program to make a Nonlinear Regression of the Antoine Equation. Use the initial guesses as shown. Plot the Graph and the Residual for this regression.

Click here for Polymath Problem Data File
File is RegressionData01.pol

OR

Click here for Polymath Solution File
File is Regression02.pol
Problem 5 – Regressions - Vapor Pressure Data

POLYMATH/Excel Solution EXERCISE

The Graph Option from the Polymath Nonlinear Regression Program indicates a reasonable representation of the data.

The Residuals Plot Option shows a more random distribution of the errors.

These graphs plus the lower variance for the Antoine equation indicate that the data are well represented.
Utilize the Export to EXCEL Option from the Polymath Regression Program to make a Nonlinear Regression of logP versus invTK. The results, shown below, are essentially the same as those obtained with Polymath. Note that the EXCEL Add-In Solver must be used to complete the Nonlinear Regression.

<table>
<thead>
<tr>
<th>T</th>
<th>logP</th>
<th>logP calc</th>
<th>logP residual</th>
<th>logP residual^2</th>
<th>logP - logP avg</th>
<th>logP(calc - logP avg)^2</th>
</tr>
</thead>
<tbody>
<tr>
<td>41.77</td>
<td>2</td>
<td>-0.4761162488</td>
<td>-2.4761162488</td>
<td>6.13136057</td>
<td>3.4042570976</td>
<td>0.368200014</td>
</tr>
<tr>
<td>56.60</td>
<td>2.30103</td>
<td>-0.235749737</td>
<td>-2.235749737</td>
<td>6.435251434</td>
<td>4.710303947</td>
<td>0.134290216</td>
</tr>
<tr>
<td>69.66</td>
<td>2.477121</td>
<td>-0.046373507</td>
<td>-2.046373507</td>
<td>6.378122507</td>
<td>5.505660738</td>
<td>0.03206967</td>
</tr>
<tr>
<td>84.78</td>
<td>2.69897</td>
<td>0.146517452</td>
<td>-2.500452548</td>
<td>6.5048608199</td>
<td>6.599577112</td>
<td>0.000317228</td>
</tr>
<tr>
<td>95.65</td>
<td>2.846008</td>
<td>0.277622193</td>
<td>-2.567475312</td>
<td>6.591032043</td>
<td>7.367520905</td>
<td>0.021564203</td>
</tr>
<tr>
<td>100.18</td>
<td>2.954243</td>
<td>0.326665467</td>
<td>-2.625577533</td>
<td>6.983667308</td>
<td>7.972550044</td>
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</tr>
<tr>
<td>114.79</td>
<td>3.079181</td>
<td>0.468270911</td>
<td>-2.595913193</td>
<td>6.736763714</td>
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<tr>
<td>123.4</td>
<td>3.176091</td>
<td>0.507850451</td>
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<td>6.802869984</td>
<td>9.274360405</td>
<td>0.19109731</td>
</tr>
</tbody>
</table>

**Solver Parameters**
- Set Target Cell: F13
- Equal To: Max
- By Changing Cells: B13
- Subject to the Constraints:
Problem 5 – Regressions - Vapor Pressure Data

The EXCEL Nonlinear Regression results obtained with Solver, shown below in spreadsheet and magnified view, are essentially the same as those obtained with Polymath.

Click here for EXCEL Solution File
File is Regression02.xls
SUMMARY - Desktop Problem Solving Involving Polymath, Excel and MATLAB

- Mathematical Model
  - Polymath 6.1
  - Solution Algorithm
- Excel Solution
  - Excel
  - Polymath Solution
  - MATLAB
  - MATLAB Solution

Happy Future Problem Solving!