Current Attributes and Future Prospects for Polymath Software

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Polymath Software – Current Information

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Three Versions

AnnualDepartmental Site License – CACHE Corporation
~60 USA ~50 Global

Educational and Professional for Individuals from POLYMATH Software

Six Textbooks

POLYMATH is usually provided on CD-ROM along with text

Newest from Prentice Hall – Authors: Cutlip and Shacham

Problem Solving in Chemical and Biochemical Engineering with POLYMATH, Excel, and MATLAB

Resolución de problemas en ingeniería química y bioquímica con Polymath, Excel y Matlab

Polymath Software – Brief History

1981 – Simulation Package marketed for the PLATO Educational System by the Control Data Corporation

1984 – Polymath Math Solver for the CDC 110 MicroPlato System

1984 – Polymath 1.0 for MS-DOS and PC-DOS marketed by CDC and introduced at the San Francisco AIChE Meeting

1990 – Polymath 2.1 site licenses marketed by CACHE Corporation followed by 3.0 in 1992, 4.0 in 1996, 5.0 in 2001 and 6.0 in 2005

www.cache.org

2001 – Polymath Educational and Professional versions marketed by Polymath Software

www.polymath-software.com

Polymath – Current Educational Version

- Operating Systems - (Windows 95 through Vista)
- Linear Equations (100)
- Nonlinear Equations (30) with Explicit Equations (40)
- Ordinary Differential Equations (30) with Explicit Equations (40)
- Regression and Curve Fitting for up to 5th degree Polynomials and 301 Data Points for Linear, Multiple Linear and Nonlinear Regressions

Polymath – Current Problem Solving Options

- **POLYMATH Problem Entry**
- **POLYMATH Problem Solution**
- **Automatic Export to Excel for Problem Solution**

  POLYMATH ODE_Solver Add-In for Excel
- **Automatic Creation of Ordered MATLAB code**

  POLYMATH Provides MATLAB Templates for m-file Creation and Problem Solution

Polymath Software – A Very Simple Example

Let's consider a simple example of a model of a well-mixed batch reactor that is described by a system of ordinary differential equations. The batch reactor initially has only reactant A. This reactant A reacts to form product B which in turn reacts to form product C. The reactions are first order and irreversible. This example will be solved with all three software packages. Often the intermediate product B is desired in a chemical process.

$$A \xrightarrow{k_1} B \xrightarrow{k_2} C$$

Ordinary Differential Equations for this Problem

The differential mass balances on a batch reactor yield three simultaneous first order ordinary differential equations and two explicit equations for the reaction rate constants:

$$\frac{dC_A}{dt} = -k_1 C_A \qquad \text{I. C. } C_A\big|_{t=0} = 1$$

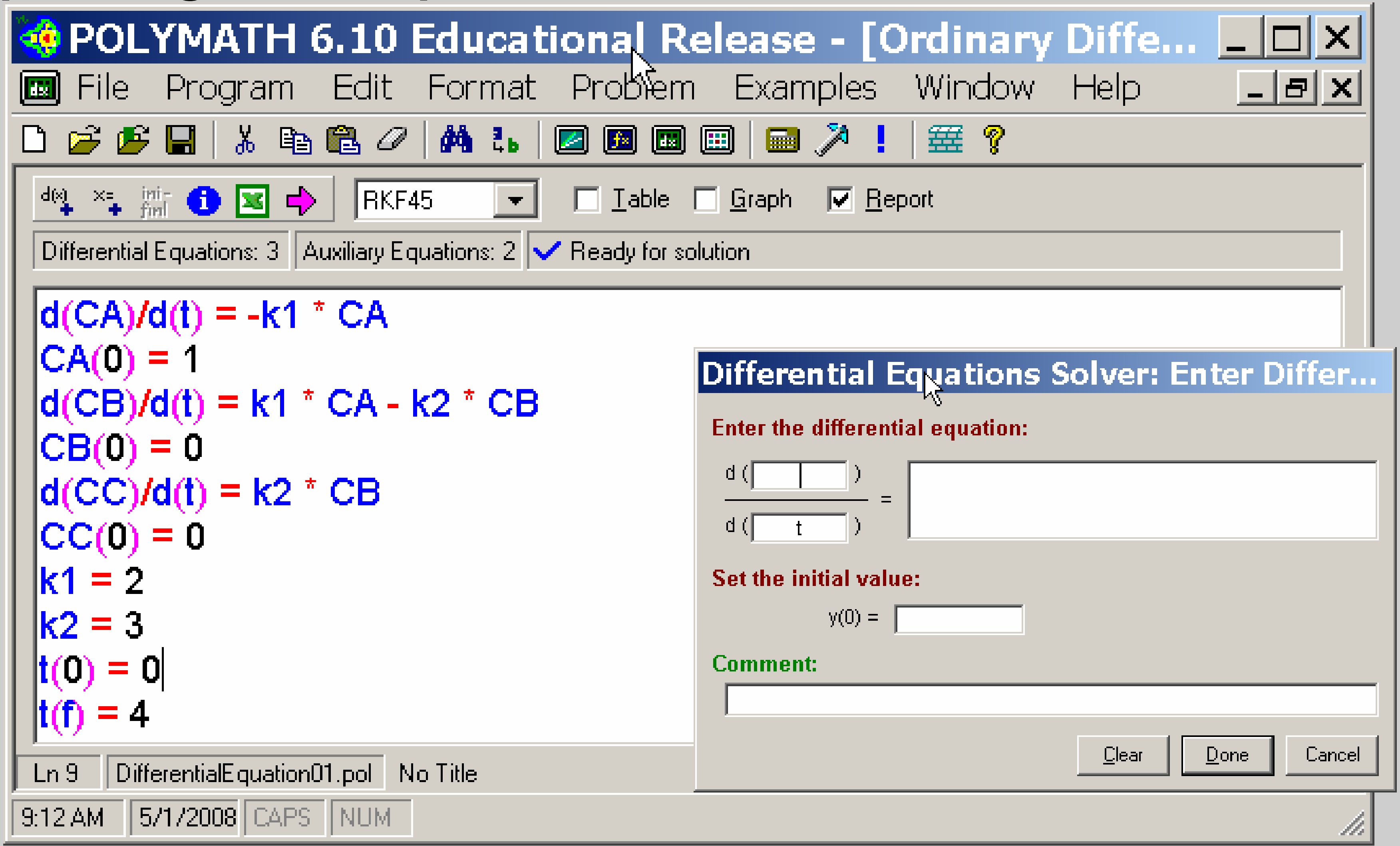
$$\frac{dC_B}{dt} = k_1 C_A - k_2 C_B \qquad \text{I. C. } C_B\big|_{t=0} = 0$$

$$\frac{dC_C}{dt} = k_2 C_B \qquad \text{I. C. } C_C\big|_{t=0} = 0$$

$$k_1 = 2 \qquad k_2 = 3$$

POLYMATH Solution – A Brief Look

The POLYMATH full screen editor facilitates equation entry by use of templates for the input of differential equations or explicit algebraic equations.



POLYMATH Solution – Report

The POLYMATH Report Summarizes the Problem Solution

POLYMATH Report
Ordinary Differential Equations

Calculated values of DEQ variables

	Variable	Initial value	Minimal value	Maximal value	Final value
1	CA	1.	0.0003355	1.	0.0003355
2	CB	0	0	0.295797	0.0006586
3	CC	0	0	0.9990059	0.9990059
4	k1	2.	2.	2.	2.
5	k2	3.	3.	3.	3.
6	t	0	0	4.	4.

Differential equations

1 d(CA)/d(t) = -k1 * CA

2 d(CB)/d(t) = k1 * CA - k2 * CB

3 d(CC)/d(t) = k2 * CB

Explicit equations

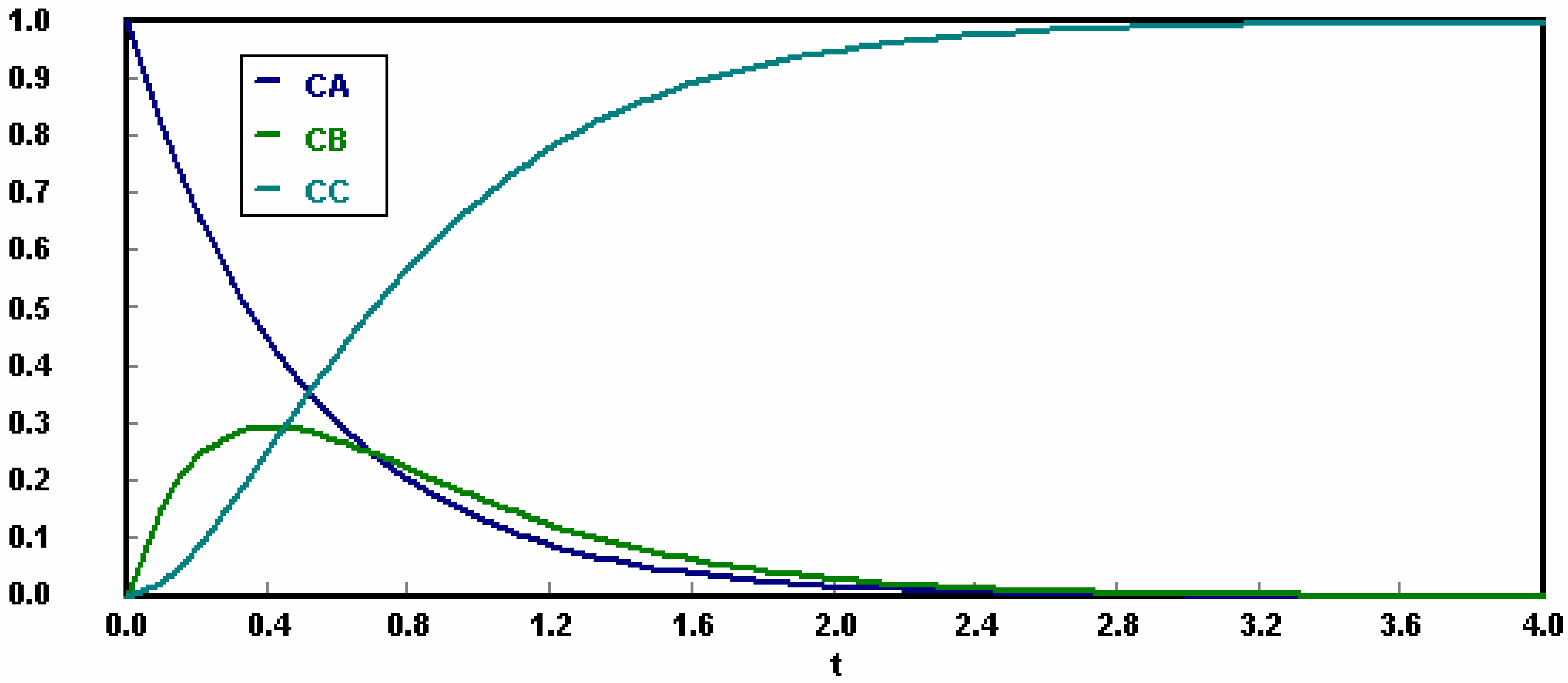
1 k1 = 2

2 k2 = 3

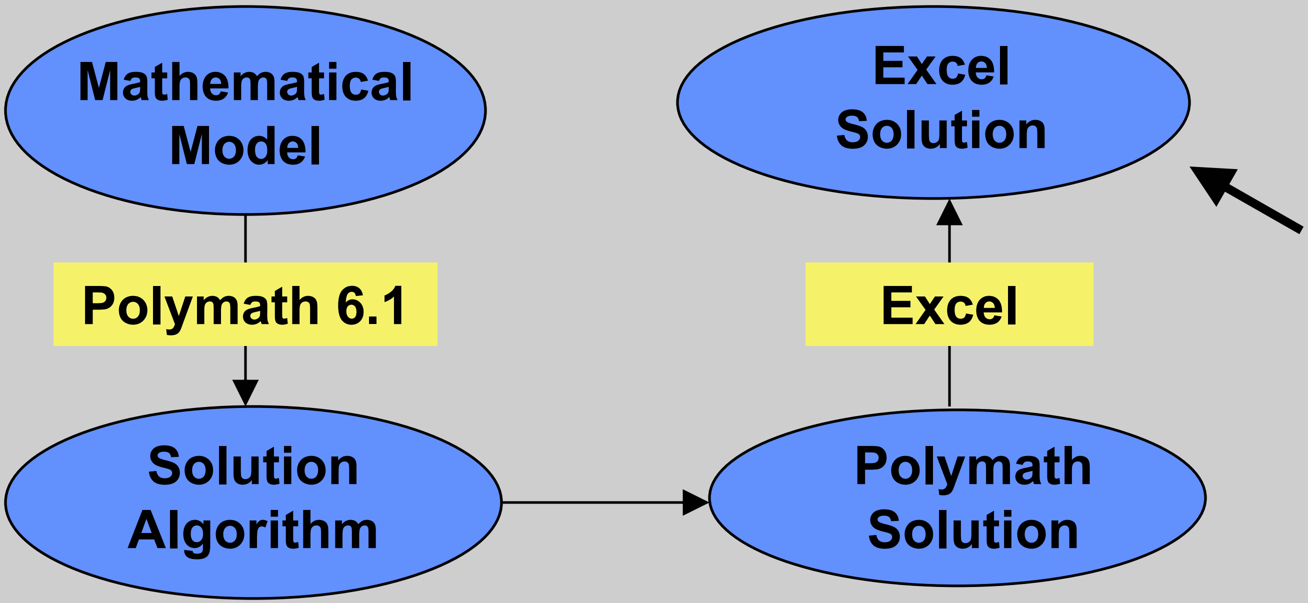
← **Report Automatically Lists Summary Table of All Variables**

← **Report Summarizes All Problem Equations**

POLYMATH Solution – Graphs



Exporting Problems from POLYMATH to Excel – A Spreadsheet is Automatically Created

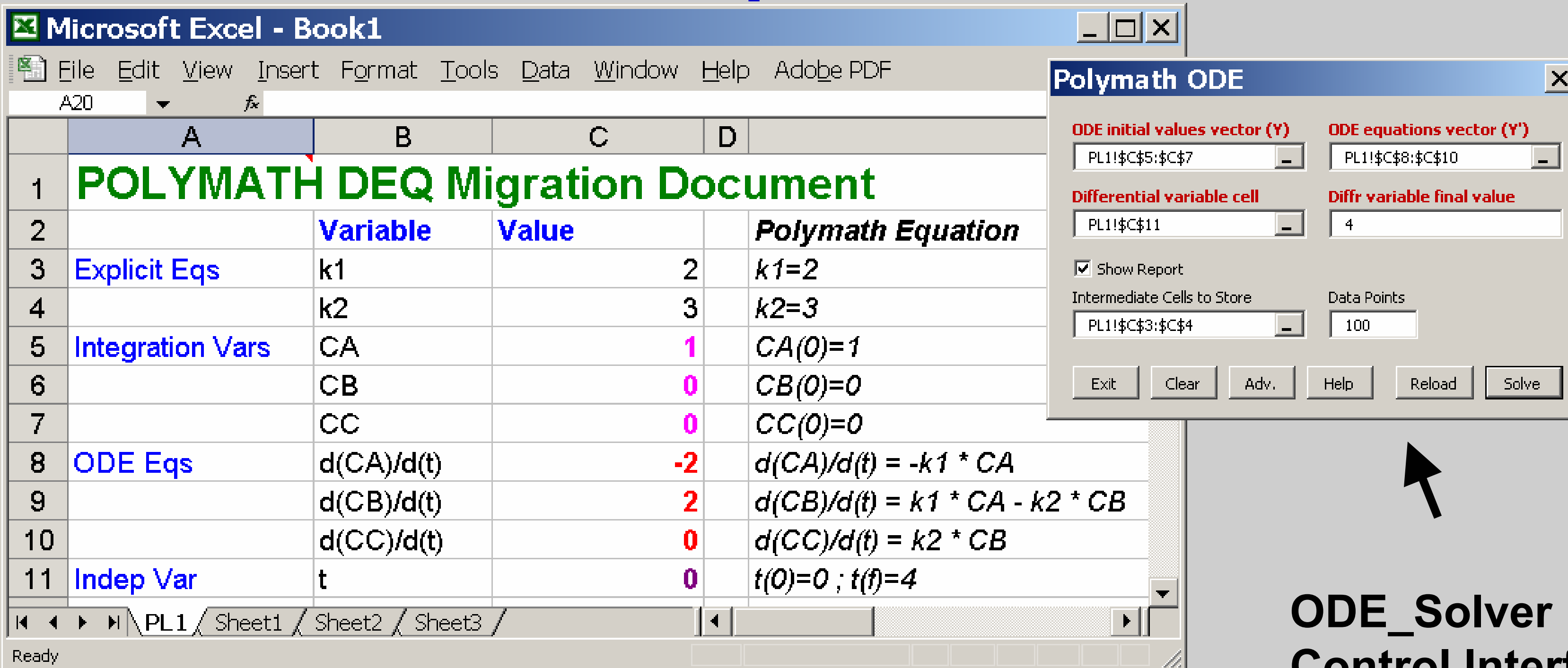


Notation and Equations Obtained from Polymath Problem Entry

ODE_Solver Add-In Available for Differential Equations

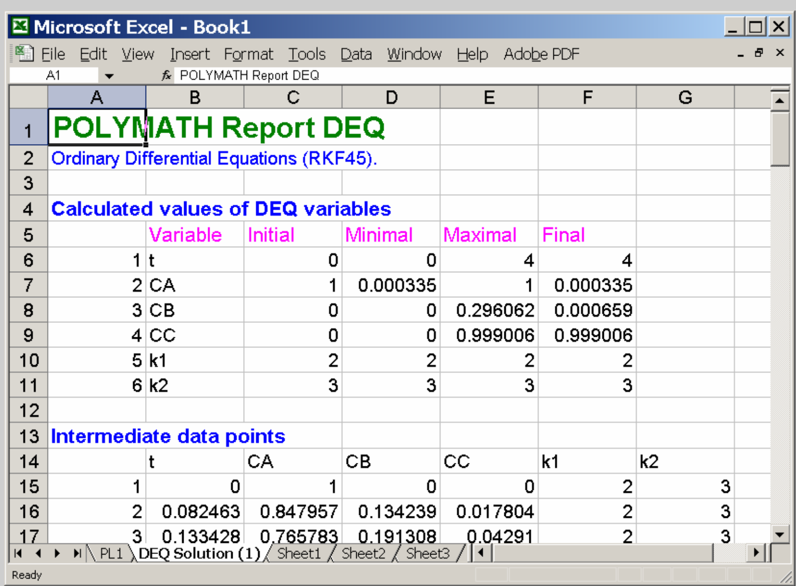
Problem Solution Automatically Displayed in New Spreadsheet

Generated Excel Spreadsheet and Solution



	A	B	C	D
1	POLYMATH DEQ Migration Document			
2		Variable	Value	Polymath Equation
3	Explicit Eqs	k1	2	k1=2
4		k2	3	k2=3
5	Integration Vars	CA	1	CA(0)=1
6		CB	0	CB(0)=0
7		CC	0	CC(0)=0
8	ODE Eqs	d(CA)/d(t)	-2	d(CA)/d(t) = -k1 * CA
9		d(CB)/d(t)	2	d(CB)/d(t) = k1 * CA - k2 * CB
10		d(CC)/d(t)	0	d(CC)/d(t) = k2 * CB
11	Indep Var	t	0	t(0)=0 ; t(f)=4

ODE_Solver Control Interface Sets Up Solution to Differential Equations

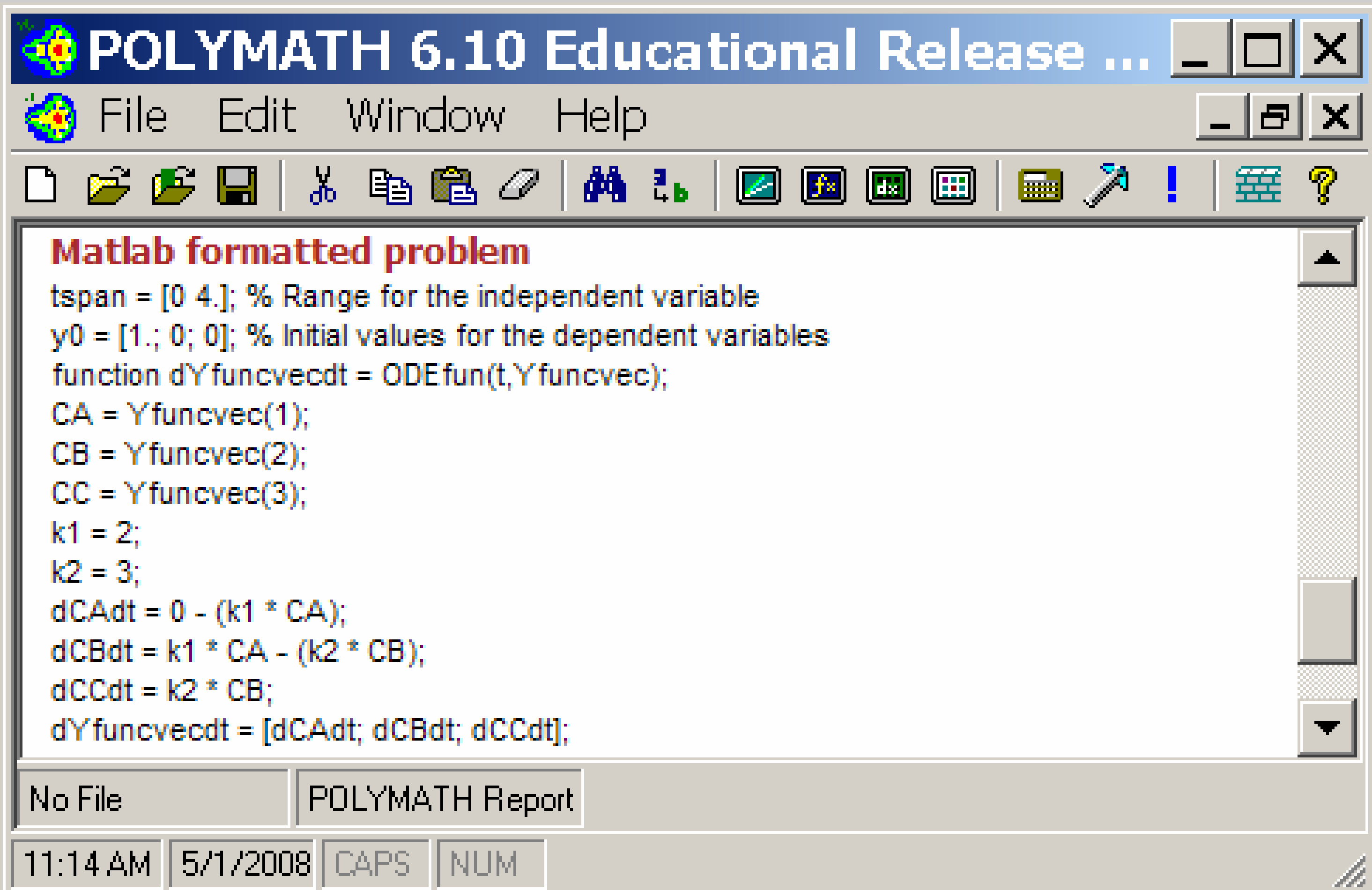


	A	B	C	D	E	F	G
1	POLYMATH Report DEQ						
2	Ordinary Differential Equations (RKF45).						
3							
4	Calculated values of DEQ variables						
5		Variable	Initial	Minimal	Maximal	Final	
6	1	t	0	0	4	4	
7	2	CA	1	0.000335	1	0.000335	
8	3	CB	0	0	0.296062	0.000659	
9	4	CC	0	0	0.999006	0.999006	
10	5	k1	2	2	2	2	
11	6	k2	3	3	3	3	
12							
13	Intermediate data points						
14		t	CA	CB	CC	k1	k2
15	1	0	1	0	0	2	3
16	2	0.082463	0.847957	0.134239	0.017804	2	3
17	3	0.133428	0.765783	0.191308	0.04291	2	3

Report of Solution is Automatically Generated in New Worksheet

Exporting Problems from POLYMATH to MATLAB for Solution – A Brief Look

POLYMATH can also output MATLAB code that automatically contains translations of the intrinsic functions and logical statements and orders the equations.

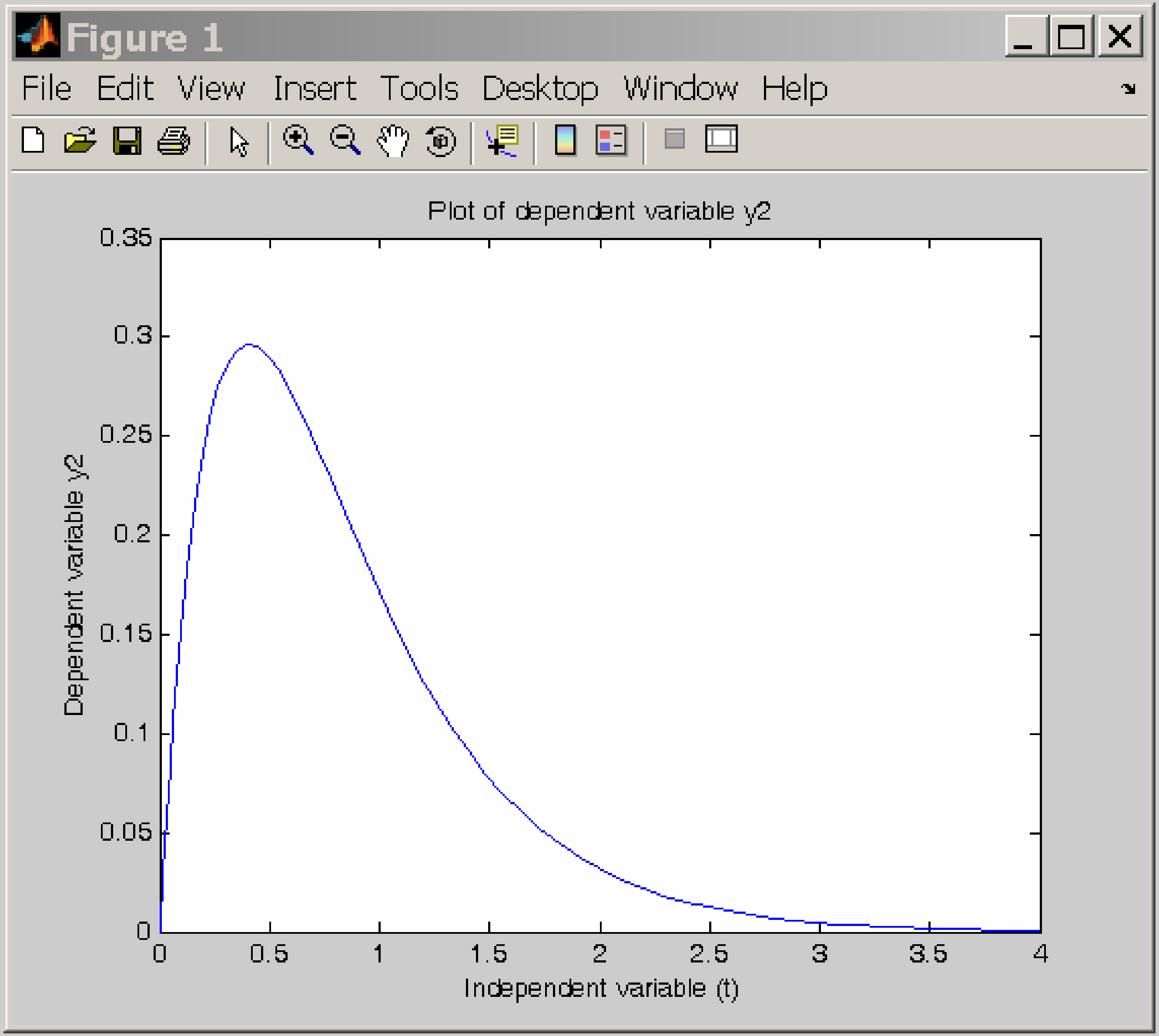


Exporting Problems from POLYMATH to MATLAB for Solution – A Brief Look

Incorporation of the generated code into a provided MATLAB Template for simultaneous ordinary differential equations gives the m-file shown where the yellow bars indicate the placement of the code generated by POLYMATH.

```
function MATLAB01
clear, clc, format short g, format compact
tspan = [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' 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(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];
```

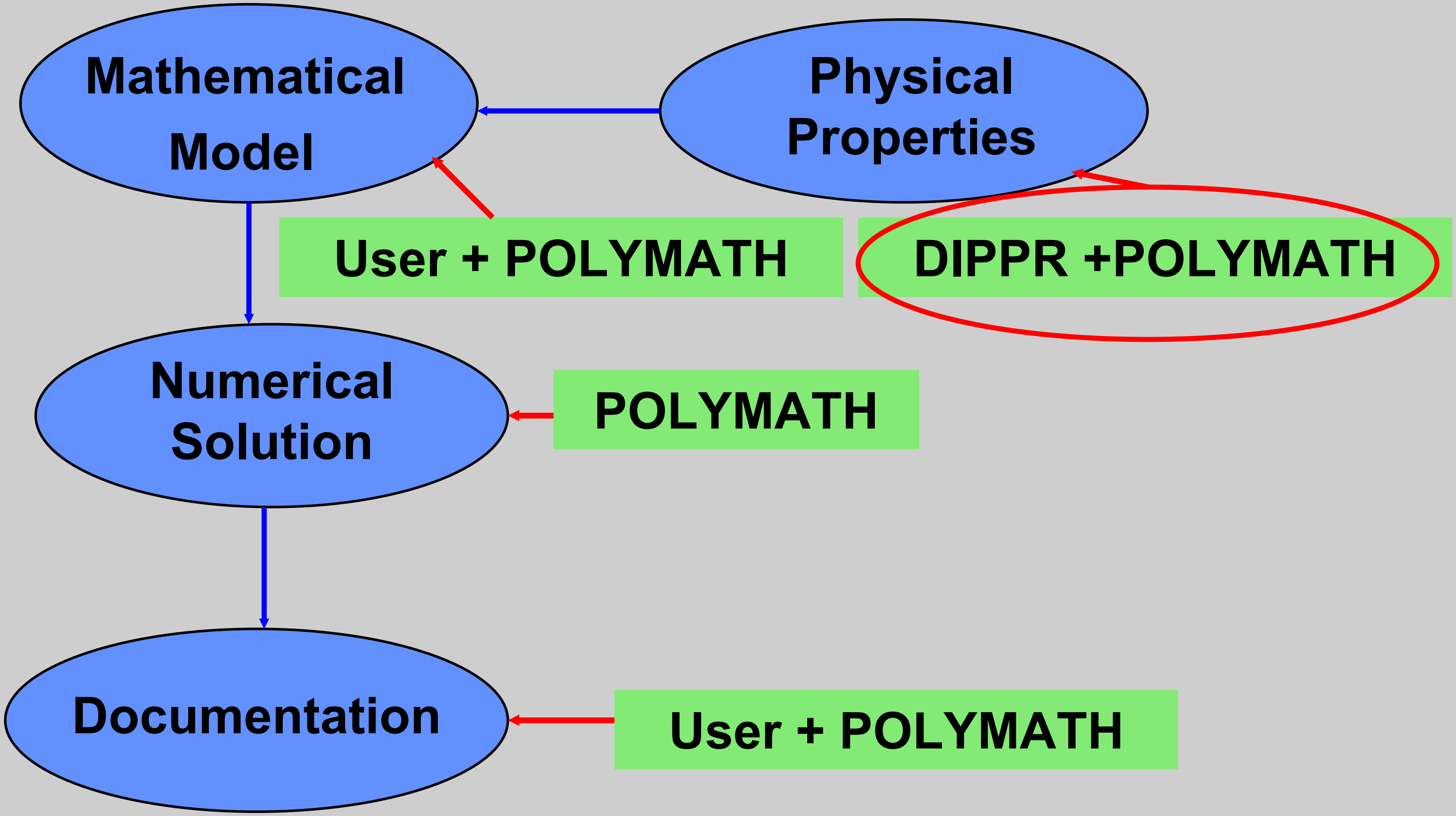
Partial Graphical Results as Generated by MATLAB for Concentration of B



Polymath Software – Possible Future Developments

- Direct Import of Physical Property Data and Correlations from DIPPR into POLYMATH
- Templates for Solving Multiple Model Multiple Algorithm (MMMA) Problems by MATLAB
- Conversion of Polymath Coding to Microsoft's .NET Framework

POLYMATH Modeling with Direct Access to the DIPPR Database



Using this approach the USER supplies the mathematical model. The physical properties are imported from DIPPR. POLYMATH rearranges the model and provides the numerical solution with partial documentation.

The DIPPR Database

DIPPR 801 Products

DIPPR 801 Database Highlights

- Contains 1944 compounds
- Lists values for 49 thermophysical properties
- Provides chemical data for 34 constant properties
- Includes 15 temperature dependent properties
- Contains raw data from the literature
- Contains critically evaluated, recommended thermophysical values
- Predicts appropriate values when experimental chemical data is not available
- References, notes, and quality codes included for all thermophysical data points

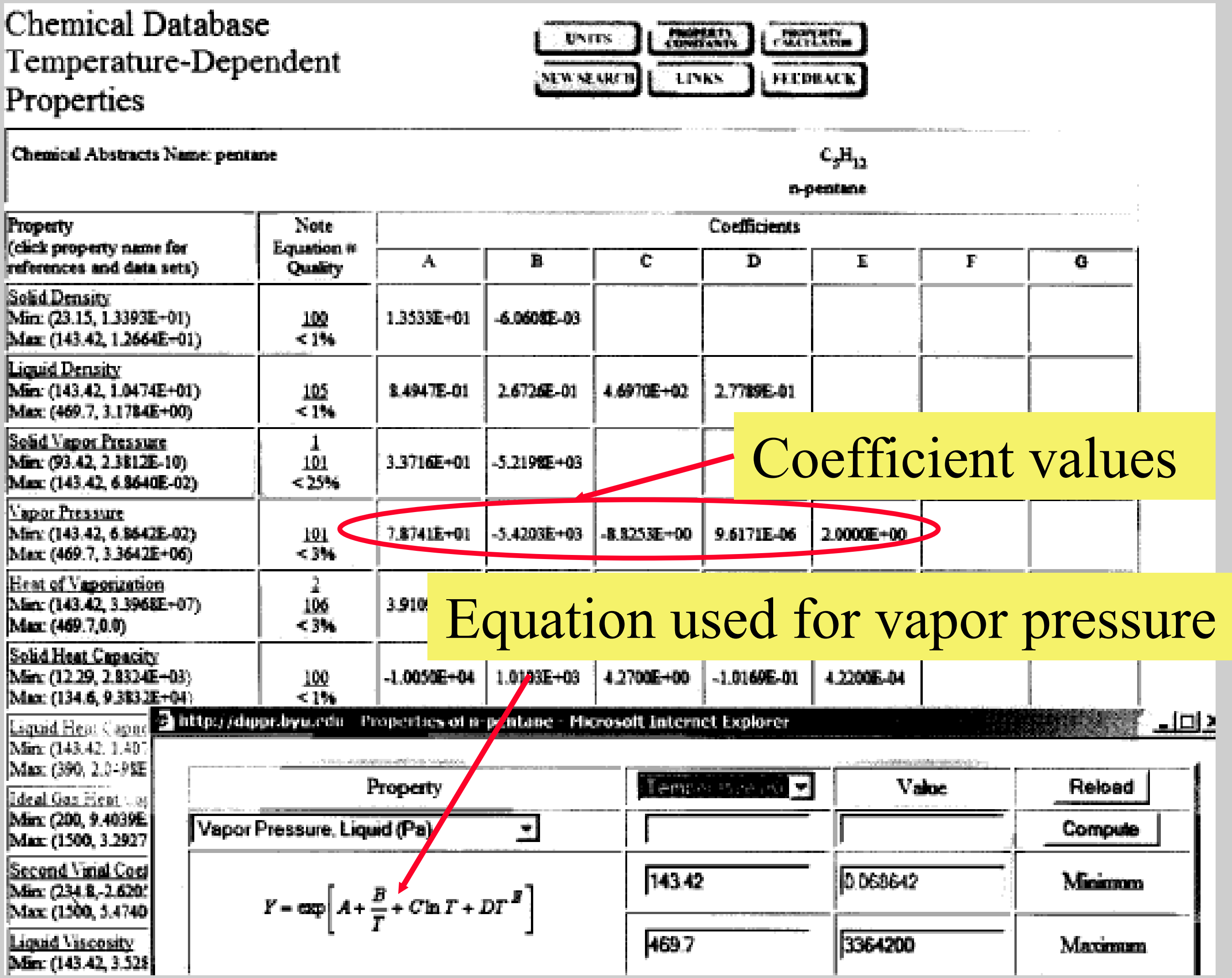
A Typical Example where Temperature Dependent Properties are Needed

Bubble Point Calculation for an Ideal Binary System

f(Tbp)=xA*PA+xB*PB-760
xA=0.1
PA=
PB=
xB=1-xA
yA=xA*PA/760
yB=xB*PB/760
Tbp(min)=30
Tbp(max)=69

The objective is to import the vapor pressure correlations (including coefficients) from DIPPR

Temperature Dependent Properties In the Web Version of the Database


Chemical Database
Temperature-Dependent
Properties

UNITS | PROPERTY CONSTANTS | PROPERTY CALCULATOR
NEW SEARCH | LINKS | FEEDBACK

Chemical Abstracts Name: pentane

C_5H_{12}

n-pentane

Property (click property name for references and data sets)	Note Equation # Quality	Coefficients A	B	C	D	E	F	G
Solid Density Min: (23.15, 1.3393E+01) Max: (143.42, 1.2664E+01)	100 < 1%	1.3533E+01	-6.0608E-03					
Liquid Density Min: (143.42, 1.0474E+01) Max: (469.7, 3.1784E+00)	105 < 1%	8.4947E-01	2.6726E-01	4.6970E+02	2.7789E-01			
Solid Vapor Pressure Min: (93.42, 2.3812E-10) Max: (143.42, 6.8640E-02)	1 101 < 25%	3.3716E+01	-5.2198E+03					
Vapor Pressure Min: (143.42, 6.8642E-02) Max: (469.7, 3.3642E+06)	101 < 3%	7.8741E+01	-5.4203E+03	-8.8253E+00	9.6171E-06	2.0000E+00		
Heat of Vaporization Min: (143.42, 3.3968E+07) Max: (469.7, 0.0)	2 106 < 3%	3.910[illegible]						
Solid Heat Capacity Min: (12.29, 2.8324E+03) Max: (134.6, 9.3832E+04)	100 < 1%	-1.0050E+04	1.0193E+03	4.2700E+00	-1.0169E-01	4.2200E-04		
Liquid Heat Capac[illegible] Min: (143.42, 1.40[illegible] Max: (390, 2.0[illegible]								
Ideal Gas Heat [illegible] Min: (200, 9.4039E[illegible] Max: (1500, 3.2927[illegible]								
Second Virial Coef[illegible] Min: (234.8, -2.620[illegible] Max: (1500, 5.4740[illegible]								
Liquid Viscosity Min: (143.42, 3.528[illegible]								

http://dippr.byu.edu Properties of n-pentane - Microsoft Internet Explorer

Property	Temperature	Value	Reload
Vapor Pressure, Liquid (Pa)			Compute
$Y = \exp\left[A + \frac{B}{T} + C \ln T + DT^E\right]$	143.42	0.068642	Minimum
	469.7	3364200	Maximum

The Bubble Point Problem with Imported Correlations

```
f(Tbp)=xA*PA + xB*PB - 760  # Bubble point temperature K
xA=0.1
PA_pa= exp(7.8741E+01-5.4203E+03/Tbp-8.8253*ln(Tbp) +9.6171E-6*Tbp^2)
# Vapor Pressure, liquid, limits: 143.42 K - 469.7 K, 0.068642 Pa-3364200 Pa
# Uncertainty < 3%
PB_pa= exp(1.0465E+02-6.9955E+03/Tbp-12.702*ln(Tbp)+1.2381E-05*Tbp^2)
# Vapor Pressure, liquid, limits: 177.83 K - 507.6 K, 0.90169 Pa-3.0449E+06 Pa
# Uncertainty < 3%
PA=0.0075006*PA_pa #Vapor Pressure mmHg
PB=0.0075006*PB_pa #Vapor Pressure mmHg
xB=1-xA
yA=xA*PA/760
yB=xB*PB/760
Tbp(min)=303
Tbp(max)=400
```

In addition to the correlations the ***units*** of the temperature and the units of the property, the ***ranges of applicability*** of the correlation and the *uncertainty* of the property are also imported

The Benefits of Direct Access from POLYMATH to DIPPR

- Using a reliable, evaluated source for all physical property needs
- Realizing that the full definition of a property includes its units and its uncertainty.
- Realizing that the full definition of a correlation includes its ranges of validity, units of the temperature and the property, and the uncertainty of the property
- Direct import of the properties saves time and reduces the chance for introducing errors or missing necessary information while using "Copy and Paste" to transfer the data from DIPPR to Polymath