POLYMATH – the History, the Present, the New DIPPR Database Option and the Future of This Popular CACHE Numerical Problem-Solving Package

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Thanks..

Leroy Stutzman – CDC Board of Directors and Professor of CHEG at UCONN (PLATO Project in Computer-based CRE Course in 1978)

David Himmelblau – Former Executive Officer of CACHE Corporation (Supporter, Exective Officer of CACHE in 1990 when POLYMATH became a CACHE Product.)

Ed Rosen – Software Task Force Leader and major supporter

Bob Seader and Brice Carnahan – Long-time supporters and users of POLYMATH

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Tom Edgar (Current Executive Officer of CACHE), Peter Rony, Robert Hesketh and CACHE Trustees

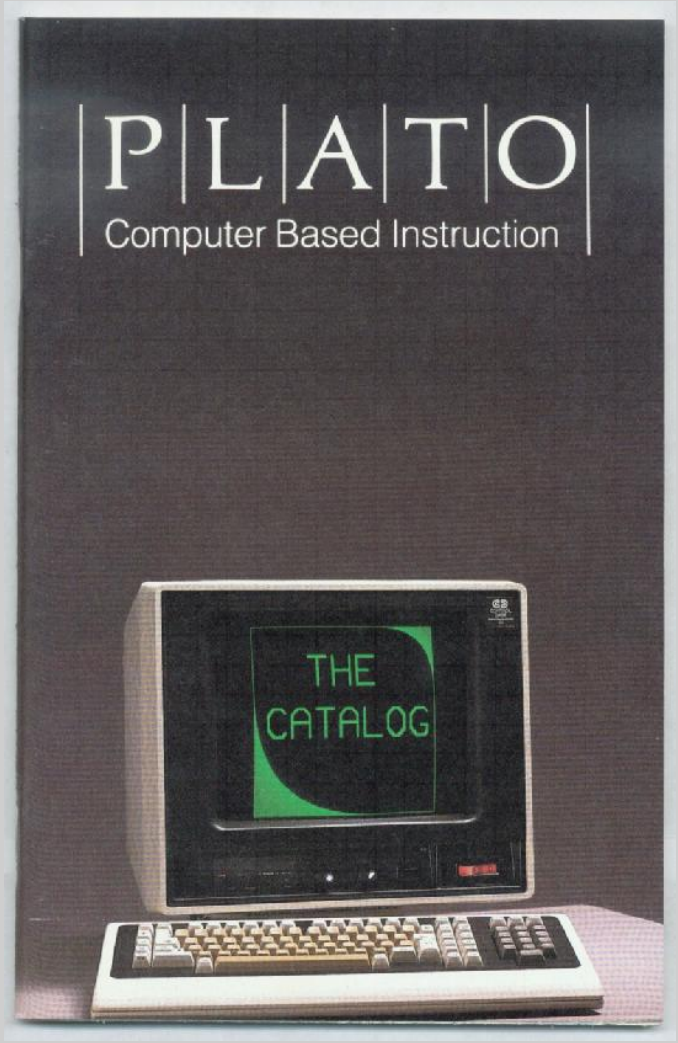
Scott Fogler and his CRE Books starting with 3rd Edition, then 4th Edition, now new 1st Edition of Essentials of CRE and David Himmelblau's Introduction to Chemical Engineering Book

Programmers: Paul Babcock, Orit Shacham, Michael Elly

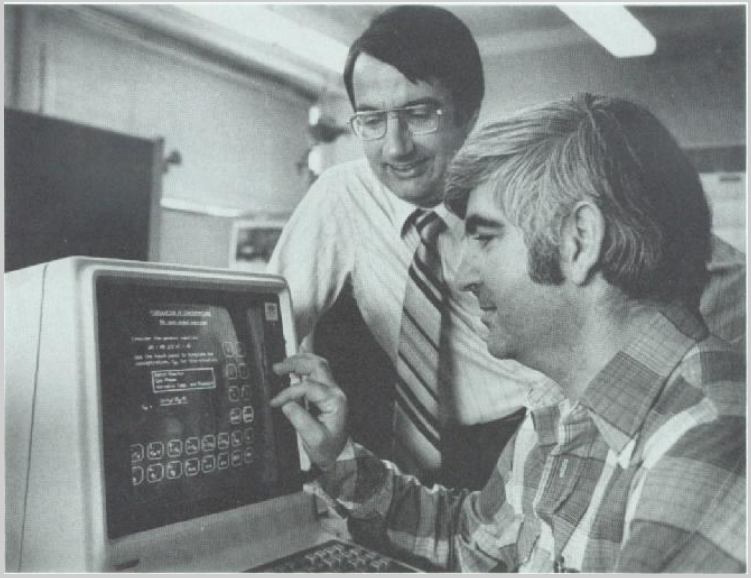
Our Home Departments and Universities… and our students with various versions of Polymath…

Our Families over our 32 years of collaboration…

Personal Calculations ~ 1980
The Control Data PLATO System



This system was in use at several Universities by Chemical Engineering Students – Illinois, Delaware, Connecticut



Personal Calculations ~ 1981
The Control Data PLATO System

Computers and Chemical Engineering Vol. 6, No. 3, pp. 209–218, 1982
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A SIMULATION PACKAGE FOR THE PLATO EDUCATIONAL COMPUTER SYSTEM

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Abstract—A simulation package has been developed for the PLATO educational computer system which allows the user to apply numerical and graphical solution techniques to small-scale problems. Current state-of-the-art numerical algorithms are used with the interactive graphic capabilities of a PLATO terminal to provide efficient problem solution in less than a minute of terminal time. Convenient entry, execution, modification, and output options are combined with on-line input error detection and extensive error messages. Although primarily intended for educational purposes, industrial users will also find this package very efficient for solving small-scale problems.

Personal Calculations ~ 1981
The PLATO System Simulation Package

Capabilities:

Ordinary Differential Equations

- **Up to 6 First Order ODEs**
- **Up to 11 Explicit Algebraic Equations**
- **Total Equations May Not Exceed 11**

Simultaneous Nonlinear Equations – Up to 6

Extended Polynomial/Nonlinear Regression Program – Up to 20 data points

Personal Calculations ~ 1981
The PLATO System Simulation Package

ORDINARY DIFFERENTIAL EQUATION SIMULATOR

The purpose of this lesson is to help you to solve systems of first-order ordinary differential equations. The system may contain up to 6 differential equations. The equations should be entered in the following form:
$dx_i/dt = f(x1, x2, \ldots, xn, t, c1, c2, \ldots)$ for $i = 1, 2, \ldots, n$

How many equations are in your system? 2 ok
Please enter your equations.
dx1/dt= c9×(1-x1)/(1+x1) ok
dx2/dt= (79.Ø636-c7×c9×(1-x1)/(1+x1))/c8 ok

How many expressions/constants do you want to define? 9
Please enter your constants/expressions.
c1= x2/1.8Ø ok
c2= » $3.75+35.7\times10^{-3}\times c1-1Ø.12\times10^{-6}\times$

Personal Calculations ~ 1981
The PLATO System Simulation Package

The equations: $dx1/dt = c9 \times (1-x1)/(1+x1)$

$dx2/dt = (79.0636 - c7 \times c9 \times (1-x1)/(1+x1))/c8$

The expressions:

$c1 = x2/1.8$

$c2 = 3.75 + 35.7 \times 10^{-3} \times c1 - 10.12 \times 10^{-6} \times c1^2$

$c3 = 5.25 + 24.2 \times 10^{-3} \times c1 - 6.88 \times 10^{-6} \times c1^2$

$c4 = 7 - .385 \times 10^{-3} \times c1 + .6 \times 10^{-6} \times c1^2$

$c5 = 8.5 \times (c1 - 298) - 5.942 \times 10^{-3} \times (c1^2 - 298^2)$

$c6 = 1.28 \times 10^{-6} \times (c1^3 - 298^3)$

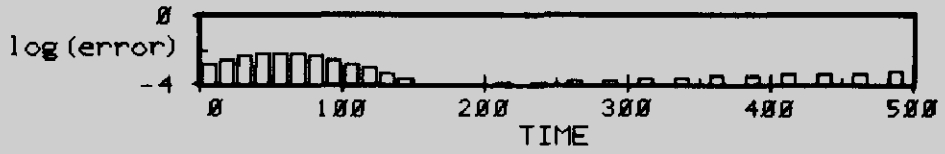
$c7 = 1.8 \times (32732 + c5 + c6)$

$c8 = (1 - x1) \times c2 + x1 \times (c3 + c4)$

$c9 = (8.54814 \times 10^{17} \times \exp(-41310/c1))/x2$

Partial results

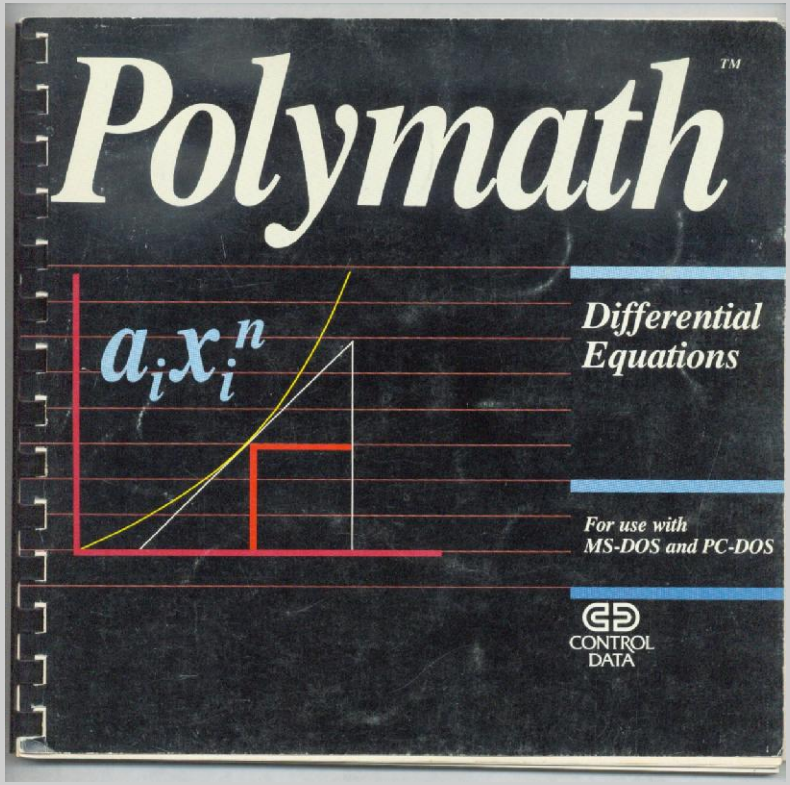
Variable	Initial value	Max. value	Min. value	Final value
t	0			500
x1	0	0.52711	0	0.52711
x2	1660	1892	1660	1892
c1	922.22	1051.1	922.22	1051.1
c2	28.066	30.093	28.066	30.093
c3	21.716	23.085	21.716	23.085
c4	7.1552	7.2582	7.1552	7.2582
c5	779.93	779.93	364.36	364.36
c6	970.09	1452.4	970.09	1452.4
c7	62068	62188	62068	62188
c8	28.066	30.225	28.066	30.225
c9	1.8113×10^{-5}	0.0038544	1.8113×10^{-5}	0.0038544



Reactor Design Problem

Personal Calculations - 1984

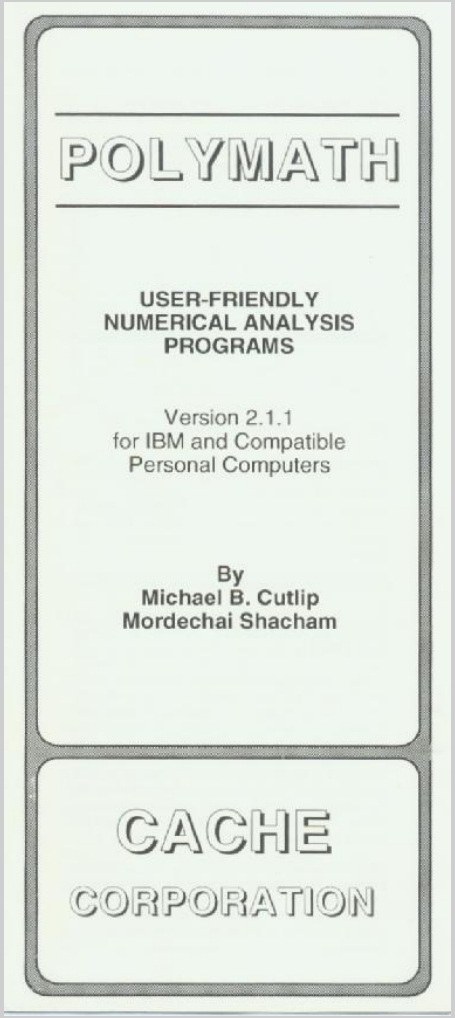
This PLATO Calculational Package became POLYMATH and a product for the IBM PC and was launched at the AIChE Annual Meeting in San Francisco in 1984

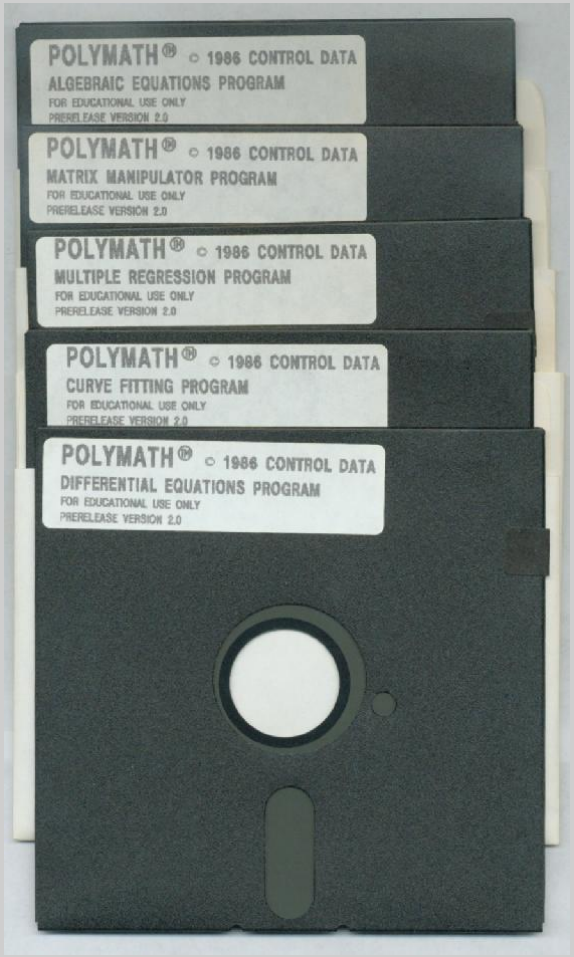


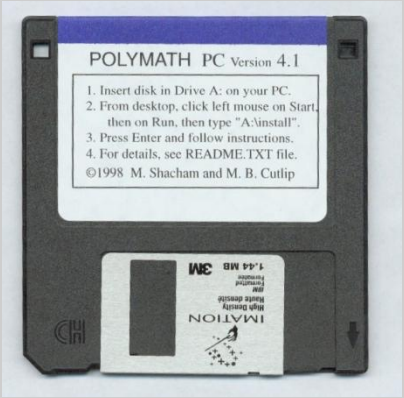
Personal Calculations - 1990

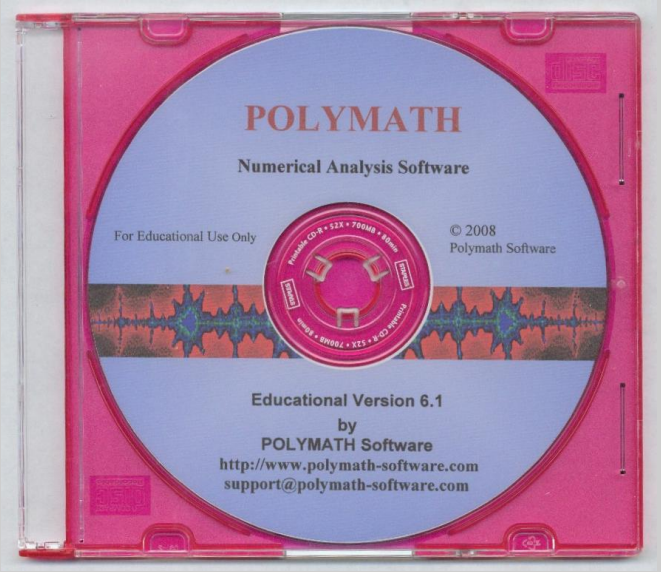
In 1990, inexpensive site licenses for POLYMATH software were first made available through the CACHE Corporation to academic departments of Chemical Engineering. Students, faculty and computer labs received personal copies on an annual basis.

POLYMATH Available from CACHE Continues









POLYMATH Today (Educational Version)

- **Linear Equations - up to 100 simultaneous equations.**
- **Nonlinear Equations - up to 30 simultaneous nonlinear and 40 explicit algebraic equations**
- **Differential Equations - up to 30 simultaneous ordinary differential and 40 explicit algebraic equations**
- **Data analysis and Regression - up to 300 data points with capabilities for linear, multiple linear, and nonlinear regressions**
- **Automatic Creation of Excel Spreadsheet Solution for Problem (include unique ODE_Solver Add-In for solving simultaneous first-order differential equations)**
- **Generation of Ordered MATLAB Code for Problem**

POLYMATH Today

- EASE OF USE WITHOUT ANY PROGRAMMING LANGUAGES OR CONTROL LANGUAGES TO REMEMBER
- FULL SCREEN EDITOR
- EXTENSIVE USER ALGORITHM SELECTION AND CONTROL
- EXECUTION WITH ALL WINDOWS OPERATING SYSTEMS (Windows 2000 – Win7 for 32 and 64 bit computers)
- COMPATIBILITY WITH PREVIOUS VERSIONS
- THREE ON-BOARD UTILITIES: POWERFUL CALCULATOR, UNIT CONVERTER, AND EXTENSIVE ENGINEERING CONVERSION FACTORS
- EXTENSIVE ON-LINE DOCUMENTATION

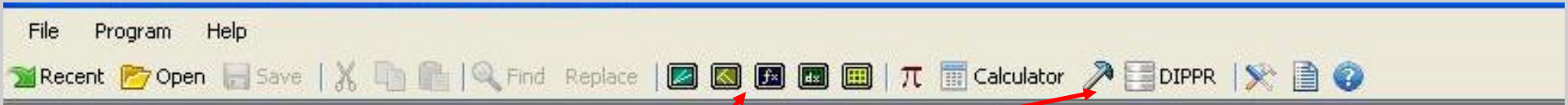
POLYMATH Current Status

- ~120 University and Departmental Site Licenses through CACHE
- Individual Educational and Professional Versions marketed by Polymath Software
- POLYMATH provided with or extensive utilized in seven textbooks for chemical engineering
- Free educational site licenses provided to department of new student chapters of AIChE for 1 + years
- Free educational site licenses are beginning to be provided to academic departments in developing countries

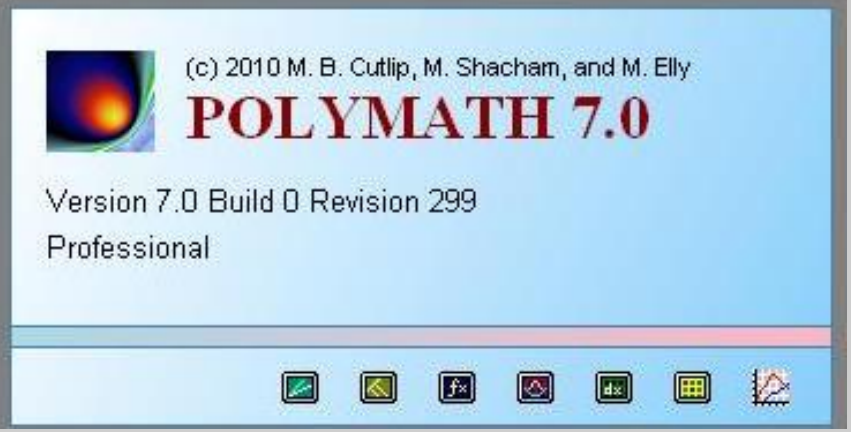
POLYMATH Current Activities

- POLYMATH 7 under development – .NET code
- Interfaces for the DIPPR Database under final development
- Search for funding support for major supported project for development and free distribution to developing countries
- Discussions with DIPPR regarding provision of limited database with POLYMATH 7
- Discussions with DIPPR regarding pricing and terms of the complete public database with POLYMATH edu site licenses as an add-on

New Features in Polymath 7.0

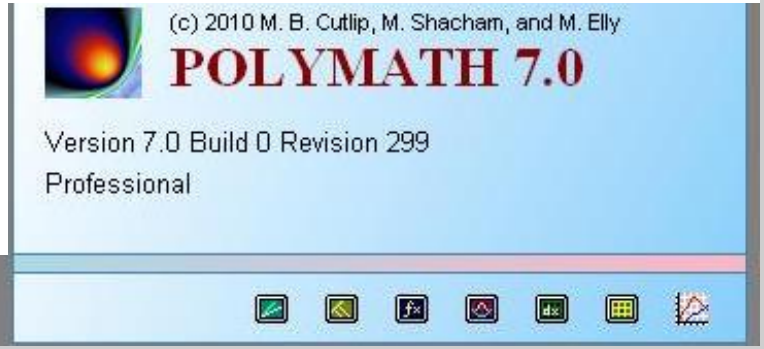


- A built in interface for the DIPPR database which contains 34 constant and 16 temperature dependent properties for ~2000 compounds
- Solution of differential-algebraic equations (ODE and NLE solvers combined)
- Solution of boundary value problems (ODEs and NLEs) solvers)
- Linear Programming
- Parameter estimation in dynamic systems (ODEs and Nonlinear Regression Programs combined)



New Features in Polymath 7.0

- ODE solver restart option (switching between stiff and non-stiff algorithms, for example)
- Option to address variable values obtained in the previous integration step in the ODE solver (for control purposes)
- Results output at an equally spaced time grid in the ODE solver
- Derivative control (?)
- User defined functions (?)



Problem Statement for Adiabatic Flame Temperature Computation

Determine the AFT for the following conditions and plot the AFT as a function of mol% CH_4 and the stoichiometric molar air to fuel ratio. The composition of natural gas is given in Table 2-15. The air-to-fuel ratios vary between 0.5 to 2.0. It can be assumed that the air and natural gas enter the burner at room temperature and atmospheric pressure. What composition and air-to-fuel ratio leads to the highest AFT?

Table 2-15 Composition of Natural Gas

Compound	mol%
CH_4	65 – 95
C_2H_6	3 – 33
N_2	2

The molar heat capacity of the reactants and the combustion products can be calculated from the equation

$$C_p^* = \alpha + \beta T + \gamma T^2 \qquad \textbf{(2-42)}$$

where T is in K and C_p^* is in cal/g-mol·K. The constants of this equation for the different components are shown in Table 2-16 as given by Smith and Van Ness.[7] The heat of combustion is -212798 cal/g-mol for CH_4 and -372820 cal/g-mol for C_2H_6, as reported by Henley.[3] Assume that both the air and the natural gas enter at the temperature of 298 K and that the N_2 content of the natural gas is

Calculation of the Adiabatic Flame Temperature

The stoichiometric equations are

$$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$$

$$C_2H_6 + 7/2O_2 \rightarrow 2CO_2 + 3H_2O$$

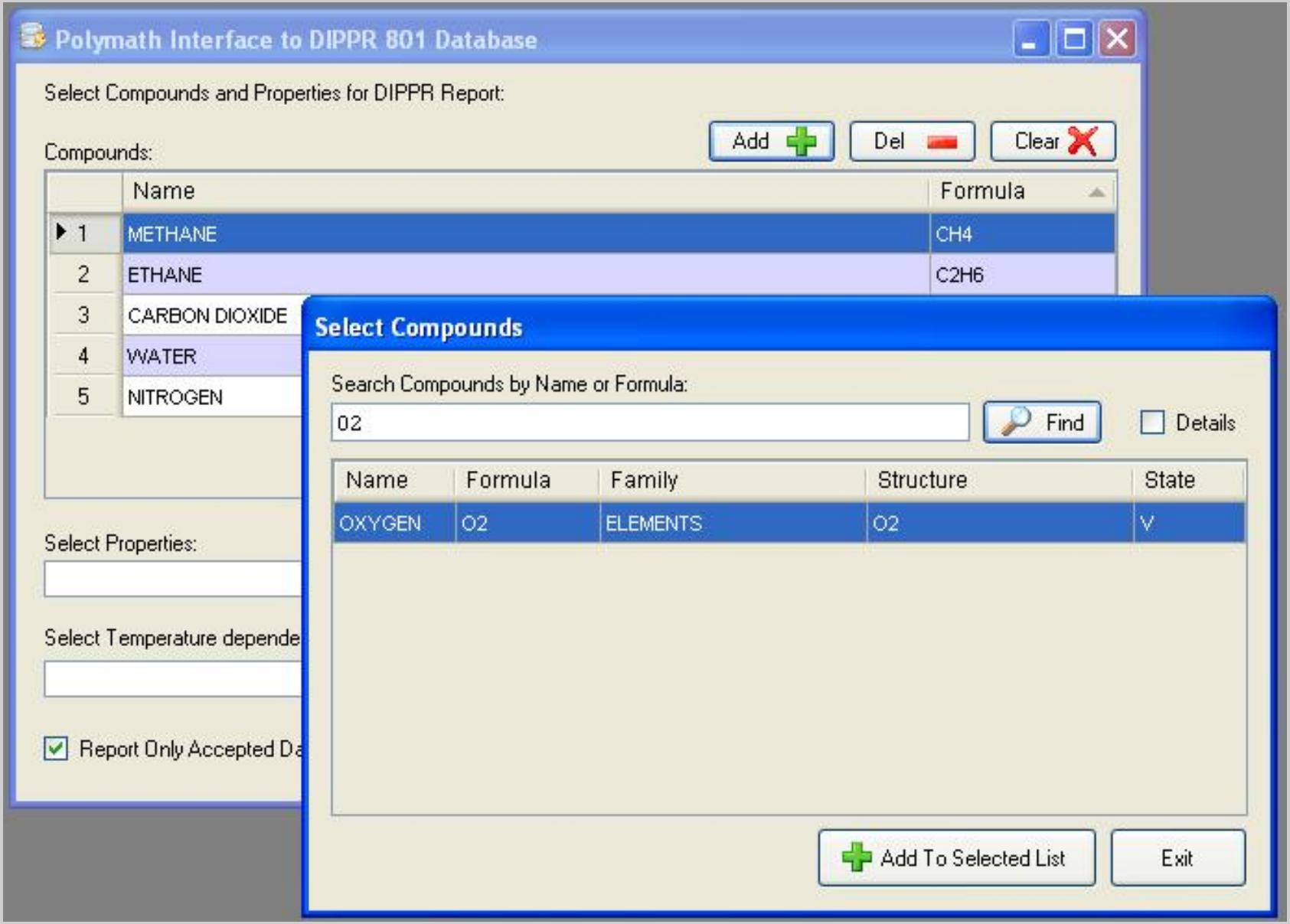
The actual to theoretical molar air-to-fuel ratio can be denoted by x with the inlet mole fractions of CH_4 and C_2H_6 denoted by y and z, respectively. For 1 mol of natural gas, there would be 0.02 mol N_2, y mol CH_4 and z mol C_2H_6. Therefore, the total moles of air required to react completely with the 1 mol of natural gas would be given by $(2y + [7 / 2]z) / 0.21$.

Material balances for the different compounds using a 1 mol natural gas basis are shown in Table 2-17 for both fuel-rich ($x < 1$) and fuel-lean ($x > 1$) situations.

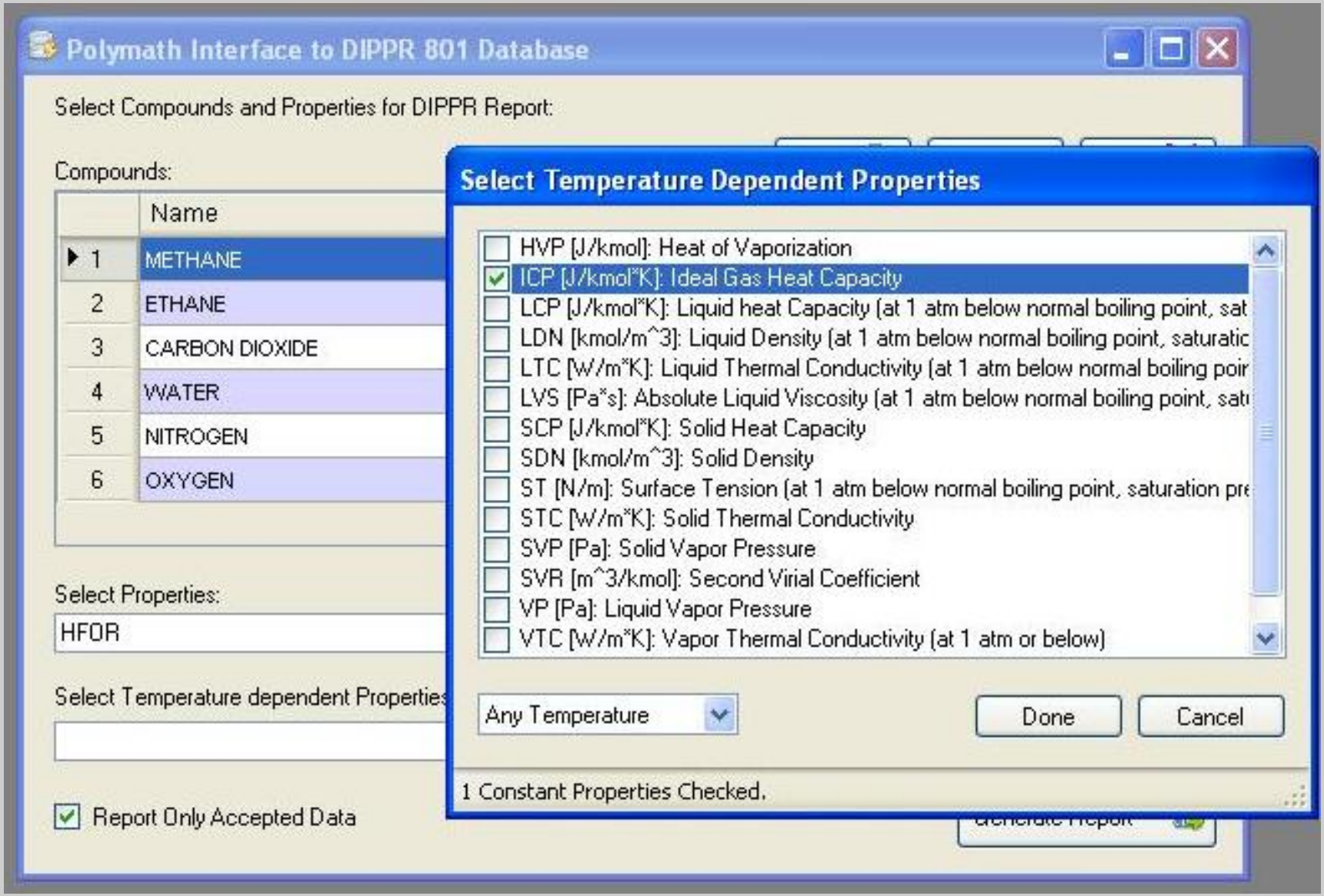
Table 2-17 Material Balance on the Reacting Species

	Moles in the product (x < 1)		Moles in the product (x > 1)	
	Expression	For $y = 0.75$	Expression	For $y = 0.75$
CH_4	$y(1-x)$	$0.75(1-x)$	0	0
C_2H_6	$z(1-x)$	$0.23(1-x)$	0	0
CO_2	$(y+2z)x$	$1.21x$	$y+2z$	1.21
H_2O	$(2y+3z)x$	$2.19x$	$2y+3z$	2.19
O_2	0	0	$\left(2y+\frac{7}{2}z\right)(x-1)$	$2.305(x-1)$
N_2	$0.02+3.76x\left(2y+\frac{7}{2}z\right)$	$0.02+8.67x$	$0.02+3.76x\left(2y+\frac{7}{2}z\right)$	$0.02+8.67x$

Selection of the Problem Compounds Using the POLYMATH 7 – DIPPR Interface



Selection of Temperature Dependent Properties Using the POLYMATH 7 – DIPPR Interface



Solving the Adiabatic Flame Temperature Problem with Polymath 7.0

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2.13 ADIABATIC FLAME TEMPERATU...

Refresh safenewt Solve

```
1  f(T) = -dHR1 * y * xx -dHR2* z * xx + H0 - Hf
2  y = 0.7
3  afr = 1.7
4  xx = if (afr<=1) then (afr) else (1)
5  z = 1 - y - 0.02
6  CH4 =  If (afr < 1) Then (y * (1 - afr)) Else (0)
7  C2H6 =  If (afr < 1) Then (z * (1 - afr)) Else (0)
8  CO2 =  If (afr < 1) Then ((y + 2 * z) * afr) Else (y + 2 * z)
9  H2O =  If (afr< 1) Then ((2 * y + 3 * z) * afr) Else (2 * y + 3 * z)
10 N2 = 0.02 + 3.76 * (2 * y + 7 * z / 2) * afr
11 O2 = if (afr<1) then (0) else ((2*y+7*z/2)*(afr-1))
12 H0 =  HIG0_CH4 * CH4 + HIG0_C2H6 * C2H6 + HIG0_CO2 * CO2 + HIG0_H2O  * H
13 Hf =HIG_CH4 * CH4 + HIG_C2H6 * C2H6 + HIG_CO2 * CO2 + HIG_H2O  * H2O + H
14 T(min) = 1000
15 T(max) = 2500
16 #T=2500
17 dHR1=HFOR_CO2+2*HFOR_H2O-HFOR_CH4 #J/kmol
18 dHR2=2*HFOR_CO2+3*HFOR_H2O-HFOR_C2H6  #J/kmol
19 T0=298.15 # K
20
21 HFOR_CH4 = -74850000 # J/kmol
22 HIG0_CH4 = 33298*T0 + 79933 *2086.9 *(coth(2086.9 / T0)) - 41602 * 991.9
23 HIG_CH4 = 33298*T + 79933 *2086.9 *(coth(2086.9 / T)) - 41602 * 991.96*(
24 #ICP_CH4 = 33298 + 79933 * (2086.9 / T / sinh(2086.9 / T)) ^ 2 + 41602 *
25
26 HFOR_C2H6 = -83820000 # J/kmol
27 HIG0_C2H6 = 40326*T0 + 134220 *1655.5* ( coth(1655.5 / T0)) - 73223 * 75
28 HIG_C2H6 = 40326*T + 134220 *1655.5* ( coth(1655.5 / T)) - 73223 * 752.8
29 #ICP_C2H6 = 40326 + 134220 * (1655.5 / T / sinh(1655.5 / T)) ^ 2 + 73223
```

Close Print Save

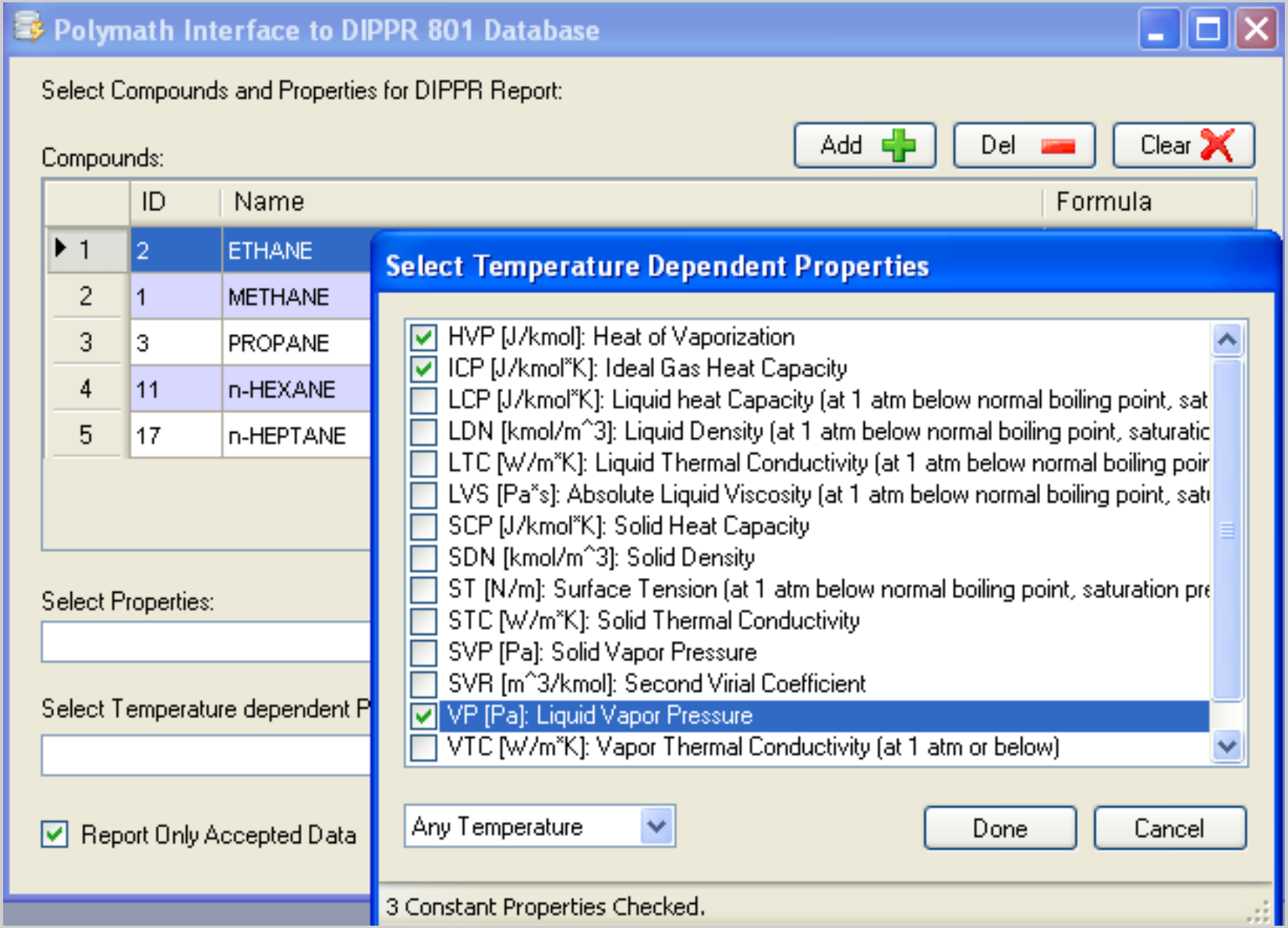
NLE Solution #1 | NLE Grf #1

Calculated values of NLE variables

	Variable	Value	f(x)	Initial Guess
1	T	1658.824	0	1750.

	Variable	Value
1	afr	1.7
2	C2H6	0
3	CH4	0
4	CO2	1.26
5	dHR1	-8.023E+08
6	dHR2	-1.429E+09
7	H0	6.028E+08
8	H2O	2.24
9	Hf	1.564E+09
10	HFOR_C2H6	-8.382E+07
11	HFOR_CH4	-7.485E+07
12	HFOR_CO2	-3.935E+08
13	HFOR_H2O	-2.418E+08
14	HIG_C2H6	3.355E+08
15	HIG_CH4	2.293E+08

Selection of the Required Property Correlation Equations by the Polymath 7- DIPPR interface



MATLAB formatted physical property equations and supporting information as generated by the Polymath 7.0 DIPPR interface

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Stack: Base

1.0 1.1

```
% Heat of Vaporization of C5H12
% n-PENTANE
% Uncertainty: < 1%; Acceptance: A; Data Type: Experimental; Source Type: Unevaluated;
% Tc=469.7
% Min_T=143.42, Max_T=469.7, Min_Val=33968000, Max_Val=0 [K ; J/kmol]
HVP_C5H12 = 39109000 * (1 - (T / 469.7)) ^ 0.38681; % J/kmol
% Ideal Gas Heat Capacity of C5H12
% n-PENTANE
% Uncertainty: < 1%; Acceptance: A; Data Type: Smoothed; Source Type: Evaluated; Sourc
% Min_T=200, Max_T=1500, Min_Val=94039, Max_Val=329270 [K ; J/kmol*K]
% HIG_C5H12 = 88050*T+301100*1650.2*coth(1650.2/T)-189200*747.6*tanh(747.6/T)+HCON %
ICP_C5H12 = 88050 + 301100 * (1650.2 / T / sinh(1650.2 / T)) ^ 2 + 189200 * (747.6 / T
% Liquid Vapor Pressure of C5H12
% n-PENTANE
% Uncertainty: < 3%; Acceptance: A; Data Type: Experimental; Source Type: Unevaluated;
% Min_T=143.42, Max_T=469.7, Min_Val=0.068642, Max_Val=3364200 [K ; Pa]
VP_C5H12 = exp(78.741 - (5420.3 / T) - (8.8253 * log(T)) + 9.6171E-06 * T ^ 2); % Pa
```