

# COMBINING NUMERICAL PROBLEM SOLVING WITH ACCESS TO PHYSICAL PROPERTY DATA – A NEW PARADIGM IN CHE EDUCATION

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*Abstract: Problem solving is an essential part of engineering education, and many educational benefits can be derived when solving realistic problems. The use of realistic problems has been hindered, so far, by the difficulty of finding reliable and consistent property data. We have developed a new approach for problem solving, which involves the use of three available packages: Polymath Numerical Computation Package<sup>®</sup> for setting up the mathematical models with a new feature to export problems to Excel<sup>™</sup>, Aspen Properties<sup>™</sup> for providing the property data via an Excel Add-In, and Microsoft<sup>™</sup> Excel for an effective solution of the problem on a widely-used platform.*

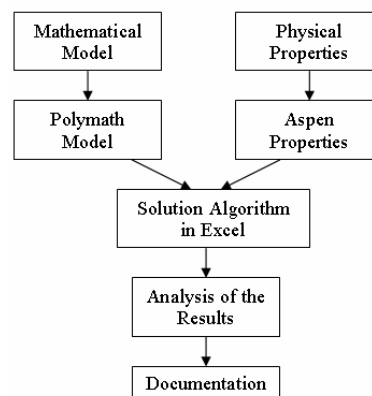
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## Introduction

Problem solving is an essential part of engineering education and is widely utilized by practicing chemical engineers. The process of problem solving within chemical engineering starts by converting the problem definition into a mathematical model using physical laws such as mass balances, energy balance, phase equilibrium relations, etc. The model is complemented by physical and thermodynamic property constants or property equations. The complete model is fed into the solution algorithm (typically a numerical solution algorithm) which provides the solution. This solution should be analyzed for physical feasibility and consistency with results of similar problems, and the model or the properties must be corrected as necessary. Finally the complete solution, including the model the property data and the results, should be verified and then documented.

## Combining Direct Access to Physical Properties with Problem Solving

A new approach to problem solving has been developed which enables real problems to be accurately solved in a time-effective manner is depicted schematically in Figure 1. It involves the use of three available packages: Polymath Numerical Computation Package (Polymath Software, <http://www.polymath-software.com>) for setting up the mathematical models with a new feature to export problems to Excel (Microsoft Corporation, <http://www.microsoft.com>), Aspen Properties (AspenTech, <http://www.aspentech.com>) for providing the property data via an Excel Add-In, and Microsoft Excel for an effective solution of the problem on a widely-used platform.



**Figure1.** Problem Solving

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The Polymath package is used to setup the problem. This approach takes full advantage of the user-friendliness of this software for entering and solving the problem. A convenient feature of Polymath allows for the automatic export of the entire problem to Excel by a single keypress. All of the equations and logical/intrinsic functions are automatically generated so that the problem can be executed completely within Excel. For problems involving differential equations, the Polymath Ode\_Solver™ Add-In provides extensive numerical integration capabilities for Excel.

The Excel spreadsheet software by Microsoft Corporation is widely used by Chemical Engineers as determined by a recent survey by the CACHE Corporation<sup>2</sup>. This software is by far the more widely used calculational tool by practicing engineers. The Excel "Solver" can be used for solving nonlinear algebraic equations. Regression problems can be solved with the Excel "LINEST" function or "Solver". Systems of ODE's (ordinary differential equations) can be integrated with the Polymath ODE\_Solver Add-In for Excel.

The Aspen Properties package which is provided with the Aspen Engineering Suite™ now provides an Add-In for Excel that can be used to provide physical property data and some other calculations (bubble points and dew points for example) to an Excel spreadsheet. Thus the property data at the needed temperature, pressure and composition values can be supplied to the mathematical model during problem solution within Excel. This combined use of Polymath for initial problem setup and export to Excel and introduction of the needed physical property data with the Aspen Properties allow Excel to solve many types of educational and industrial problems.

### An Example Problem – Calculation of Adiabatic Flame Temperature<sup>1,3</sup>

This problem involves the calculation of the adiabatic flame temperature when burning natural gas of various methane-ethane-air ratios. The problem solution requires: a) preparation of the model based on material and energy balances, b) standard heat of combustion data for methane and ethane, c) ideal gas heat capacity correlations for the six compounds involved, and d) the solution of a nonlinear algebraic equation using a numerical technique.

#### 1. Polymath Solution Using Heat Capacity Correlations

The model equations for this problem, as they are entered into Polymath for one set of parameter values are partially shown in Figure 2. The Polymath equations and comments provide clear documentation of the

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POLYMATH 6.0 Educational Release - [Nonlinear Equations Solver]
File Program Edit Format Problem Examples Window Help
safenewt Graph
Nonlinear Equations: 1 Auxiliary Equations: 16 Ready for solution
f(T) = 212798 * y * xx + 372820 * z * xx + HD - Hf # Adiabatic flame temperature (K)
y = 0.75 # Inlet mole fraction of methane
x = 0.5 # Actual to theoretical molar air-to-fuel ratio
z = 1 - y - 0.02 # Inlet mole fraction ethane
O2in = 2 * y + 7 * z / 2 # Inlet moles of oxygen
O2 = If (x < 1) Then (0) Else ((2 * y + 7 * z / 2) * (x - 1)) # Moles of oxygen in the combustion gases
CH4 = If (x < 1) Then (y * (1 - x)) Else (0) # Moles of methane in the combustion gases
C2H6 = If (x < 1) Then (z * (1 - x)) Else (0) # Moles of ethane in the combustion gases
CO2 = If (x < 1) Then ((y + 2 * z) * x) Else (y + 2 * z) # Moles of carbon dioxide in the combustion gases
H2O = If (x < 1) Then ((2 * y + 3 * z) * x) Else (2 * y + 3 * z) # Moles of water vapor in the combustion gases
N2 = 0.02 + 3.76 * (2 * y + 7 * z / 2) * x # Moles of nitrogen in the combustion gases

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Figure 2. Partial Polymath Problem Entry

problem as meaningful variable names can be used. The equation form and syntax is almost identical to the mathematical form. A single mouse click on the purple icon in Polymath yields the problem solution with minimal time and effort required on the part of the user.

## 2. Export to Excel Using Heat Capacity Correlations

A single keypress in Polymath can also export a Polymath problem to Excel as a new worksheet in a previously opened workbook as shown in Figure 3 where all intrinsic and logical functions are automatically converted.

	A	B	C	D	E	F
1	<b>POLYMATH NLE Migration Document</b>					
2		<b>Variabl</b>	<b>Value</b>		<b>Polymath Equation</b>	<b>Comments</b>
3	Explicit Eqs	y	0.75		y=0.75	Inlet mole fraction of methane
4		x	0.5		x=0.5	Actual to theoretical molar air-to-fuel ratio
5		z	0.23		z=1 - y - 0.02	Inlet mole fraction ethane
6		O2in	2.305		O2in=2 * y + 7 * z / 2	Inlet moles of oxygen
7		O2	0		O2=If (x < 1) Then (0) Else ((2 * y + 7 * z / 2) * (x - 1)	Moles of oxygen in the combustion gases
8		CH4	0.375		CH4=If (x < 1) Then (y * (1 - x)) Else (0)	Moles of methane in the combustion gases
9		C2H6	0.115		C2H6=If (x < 1) Then (z * (1 - x)) Else (0)	Moles of ethane in the combustion gases
10		CO2	0.605		CO2=If (x < 1) Then ((y + 2 * z) * x) Else (y + 2 * z)	Moles of carbon dioxide in the combustion gases
11		H2O	1.095		H2O=If (x < 1) Then ((2 * y + 3 * z) * x) Else (2 * y +	Moles of water vapor in the combustion gases
12		N2	4.3534		N2=0.02 + 3.76 * (2 * y + 7 * z / 2) * x	Moles of nitrogen in the combustion gases
13		alp	41.6326516		alp=3.381 * CH4 + 2.247 * C2H6 + 6.214 * CO2 + 7.	Sum of alpha(i)*n(i)
14		bet	25.407255		bet=18.044 * CH4 + 38.201 * C2H6 + 10.396 * CO2	Sum of alpha(i)*10^3*n(i)
15		gam	-4.7223284		gam=-4.3 * CH4 - 11.049 * C2H6 - 3.545 * CO2 + 0.	Sum of gamma(i)*10^6*n(i)
16		H0	13493.0065		H0=alp * 298 + bet * 0.001 * 298 * 298 / 2 + gam * f	
17		Hf	121486.937		Hf=alp * T + bet * 0.001 * T ^ 2 / 2 + gam * 1e-6 * T .	
18		xx	0.5		xx=If (x <= 1) Then (x) Else (1)	Conversion
19	Implicit Vars	T	2000		T(0)=2000	Adiabatic flame temperature (K)
20	Implicit Eqs	f(T)	14679.6191		f(T)=212798 * y * xx + 372820 * z * xx + H0 - Hf	
21						

Figure 3. Problem Exported from Polymath to Excel

In the worksheet, the variable names, the Polymath equations, and the comments are shown for documentation purposes. The Excel formulas are generated and placed in the 3rd column, marked as "Value". They are transparent to the user unless a particular cell is examined.

## 3. Enthalpy Calculations Using Aspen Properties Software within Excel

The introduction of physical property data is enabled within the Excel spreadsheet by the use of Aspen Properties which is a part of the Aspen Engineering Suite. The data can be provided to Excel with an Add-In created with the Aspen Properties software. Thus in this case, it is useful to obtain the pure component and mixture enthalpy values at the feed and the final temperatures from the Aspen Properties Add-In. A portion of the spreadsheet that can be used to provide the needed physical property data as indicated in Figure 4.

B14    =MixtureProperty(BB:G8,B13:G13,A14,B15,K5,"V")							
	A	B	C	D	E	F	G
1							
2	<b>Computation of Adiabatic Flame Temperature</b>						
3							
4	C:\Program Files\AspenTech\Aspen Properties 12.1\Engine\req\adb_flame.aprbkp						
5							
6	<b>Global Units Set: Metrics</b>						
7							
8		<b>METHA-01</b>	<b>ETHAN-01</b>	<b>CARBO-01</b>	<b>WATER</b>	<b>OXYGE-01</b>	<b>NITRO-01</b>
9	<b>Moles in</b>	0.7500	0.2300	0	0	1.1525	4.3534
10	<b>Mole fraction</b>	0.1156	0.0355	0	0	0.1777	0.6712
11	<b>enthalpy</b>	-2770.2045	-17967.2694				
12	<b>Moles out</b>	0.3750	0.1150	0.605	1.095	0	4.3534
13	<b>Mole fraction</b>	0.0573	0.0176	0.0925	0.1673	0.0000	0.6653
14	<b>enthalpy</b>	-2745.8613	-17967.2689				

Figure 4. Table from Aspen Properties Add-In Providing Physical Property Data to Excel

This part of the Excel solution spreadsheet provides the needed physical properties as the temperature and composition change during the problem solution. The Excel equations generated by Polymath for the problem can be modified to utilize the physical property data from the cells generated by the Aspen Properties.

For this example problem, the molar enthalpy of the inlet gases is calculated in cell B11 and that of the combustion gases is calculated in cell B14. The function call to calculate the enthalpy of the combustion gases from the Aspen Properties Add-In is:

MixtureProperty(B8:G8,B13:G13,A14,B15,K5,"V")

The first parameter of this function is the list of the compounds involved, the second parameter is the list of the mole fractions of the various components, the third parameter is the name of the desired property, the fourth is the temperature, the fifth is the pressure and the last parameter is indication of the phase condition. The number of moles of the various compounds at the inlet and outlet are retrieved from the material balance equations in the spreadsheet. In this example, the Solver Add-In of Excel can then be used to calculate adiabatic flame temperature for one set of parameter values. This is shown in Figure 5.

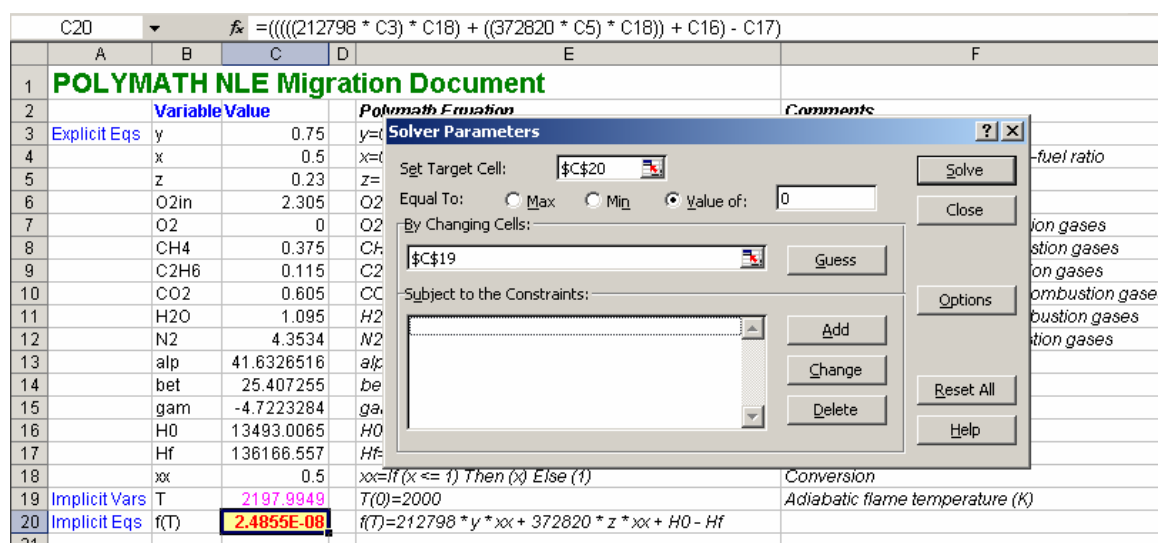


Figure 5. Adiabatic Flame Temperature Calculation

### Conclusions:

Realistic problem solving can now be efficiently conducted with the combined use of three software programs: Polymath, Excel, and Aspen Properties. This approach concentrates the creation of the needed problem equations within Polymath, which is a very user-friendly package that also allows automatic export of the problem to a commonly-used spreadsheeting package – Excel. The required physical property data can be introduced into the Excel problem solution via an Aspen Properties which is widely available in academia and industry. The actual problem is solved in Excel and solution verification can be achieved by comparing the Polymath and Excel solutions for simple cases of constant physical properties.

This approach to problem solving can be introduced as early as in the first course in Chemical Engineering. Problem solving with convenient access to physical property data can be used throughout the curriculum. This may very well represent the next paradigm shift in Chemical Engineering education. This approach can also be used in industrial practice where efficient solutions to realistic problems are frequently required.

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