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© for setting up the mathematical models with a new feature to export problems to Excel™, Aspen Properties™ 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.

The new approach is demonstrated by solving a sample problem involving calculation of an adiabatic flame temperature. It is shown that the availability of reliable and consistent property data enables instructors to replace artificial problems dealing with, say, compounds A, B and C with realistic problems dealing with real compounds. Furthermore, many different versions of the same problem can be prepared with minimal effort, as needed for exams and homework assignments. Realistic problems can be assigned routinely, as several steps of the problem solving process can be carried out very fast with the computer based tools provided, while the student concentrates his/her efforts on the subject matter and the solution options that are required.

Introduction

Problem solving is an essential part of engineering education. The best way to demonstrate mastery of the material learned is to correctly solve real-life problems associated with that material and critically analyze the results. The importance of the solution of real-life problems in chemical engineering education has been recognized long time ago. The CACHE Corporation (Computer Aids for Chemical Engineering Education) published a seven volume set of books entitled "Computer Programs for Chemical Engineering Education" in 1972 where realistic problems, involving computer solution, were provided in seven curriculum areas. At that time, however, the preparation of such problems by the instructor and their solution by the students required considerable effort and time, and thus the solution of realistic problems could be assigned very infrequently.

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The process of problem solving within chemical engineering can be represented schematically by the flow diagram shown in Figure 1. The process 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 documented.

In most courses it is not necessary to carry out all the steps of the solution process in detail in order to gain most or all the educational benefits of problem solving. Typically the preparation of the mathematical model and critical analysis of the results should be carried out in detail, while the technical details of the solution algorithm and the collection of the physical property values and correlations may be non-essential for understanding the course material. However, a critical analysis of the results requires reaching the solution and to reach the solution all the steps of the problem solving process must be carried out. Thus, in order to use problem solving effectively, the various stages of the solution process must be analyzed, and efficient tools must be provided to carry out the tasks which are not essential to the understanding of the course material.

In 1990 we revised the Polymath program (Copyrighted by M. Shacham, M. B. Cutlip and M. Elly, http://www.polymath-software.com) to enable numerical solution techniques to be applied to engineering and scientific problems while requiring minimal effort on behalf of the user with regard to the technical details of the numerical solution. This package, updated many times, continues to available to academic departments under inexpensive site licenses from the CACHE Corporation. Polymath was immediately integrated into chemical engineering problem solving as demonstrated by Fogler's[2] "French Menu of problem solving in chemical reaction engineering" shown in Figure 2. The introduction of Polymath considerably reduced the time and effort required for solving realistic problems that required numerical solutions. As a result, complex problems are now being routinely assigned in various curricular areas. This development was described by Fogler[2] as a "paradigm change in engineering education".

The accessibility of the property data and correlations has improved considerably over the years but the collection of such information is still a lengthy and error prone process as the data for various compounds and properties may be available in different databases with inconsistent units. Current educational practice is to provide the data for the problem in hand in order to prevent the students from spending too much time on searching for the data, an activity which usually does not contribute to the study of the subject matter. However, this makes the problem solving experience incomplete because the professional engineer must collect all the pertinent data before attempting to solve the actual problem. Furthermore, instructors often prefer to assign artificial problems because of the difficulty and effort required in finding reliable and consistent physical properties for real substances.

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Combining Direct Access to Physical Properties with Problem Solving

In order to enable realistic, accurate, and time-effective educational problem solving, we have developed a new approach to problem solving. The new approach is depicted schematically in Figure 3. It involves the use of three available packages: Polymath Numerical Computation Package for setting up the mathematical models with a new feature to export problems to Excel (Trademark of Microsoft Corporation, http://www.microsoft.com), Aspen Properties (Aspen Properties is a registered product of 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.

The Polymath package is used to setup the problem. This takes full advantage of the user-friendliness of this software for entering the problem and verifying its solution. A new feature of Polymath 6.0 allows 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 Aspen Properties package which is provided with the Aspen Engineering Suite™ supplies 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.

The numerical solutions are accomplished completely within Excel. The Excel "Solver" can be used for solving nonlinear algebraic equations. Regression problems utilize the Excel “LINEST” function or “Solver”. Systems of ODE’s (ordinary differential equations) use the Polymath ODE_Solver Add-In for Excel.

An Example Problem – Calculation of Adiabatic Flame Temperature (AFT)

This problem involves the calculation of the adiabatic flame temperature when burning natural gas of various methane-ethane-air ratios. The problem is based on similar problems presented by Sandall[3] and Cutlip and Shacham[1]. The complete problem definition is in Appendix A.

The problem solution in this case 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. Sandall[3] assigned this problem in a sophomore stoichiometry course where the students were expected to carry out all the steps of the problem solution using a FORTRAN program. Clearly, this problem would also be appropriate for a thermodynamics course or a course where the numerical methods could be examined in more detail.

The introduction of a user-friendly mathematical software package, such as Polymath, greatly simplifies the entry of the problem and the programming of the detailed numerical solution.

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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 shown in Figure 4. The Polymath equations and comments provide a clear documentation of the 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. The default solution algorithm solves most problems. A representative solution is given in Figure 5.

2. Polymath Export to Excel Using Heat Capacity Correlations

A single keypress in Polymath 6.0 can export a Polymath problem to Excel as shown for this example problem in Figure 6. The Excel problem appears within Excel as a new worksheet in a previously opened workbook as shown in Figure 7.

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 he/she asks explicitly to see them. The formula to calculate H_2O for example is:

$$=IF((C4 < 1),(((2 * C3) + (3 * C5)) * C4),((2 * C3) + (3 * C5)))$$

This demonstrates the importance of the use of Polymath as the model input tool, as conversion of the variable names to cell addresses makes the model input a tedious and error prone process. Furthermore, the model equations (Excel formulas) cannot be used as documentation, and such documentation must be added separately.

The solution of this problem involving a single nonlinear equation within Excel can be accomplished by the use of either Goal Seek or Solver from the Tools menu. For this problem, the Solver will be used to minimize the nonlinear equation in cell C20 by adjusting the AFT in cell C19. This is shown in Figure 8. Note that the Excel solution yields an AFT of 2017.9949 as compared to the Polymath solution which yielded an AFT of 2017.995 which is excellent agreement between the two numerical solutions. Note that Solver in Excel is useful for simultaneous nonlinear equations, while Goal Seek would be useful for only a single nonlinear equation.

3. Enthalpy Calculations Using Excel Properties

If the problem to be used in the stoichiometry or numerical methods course, or in the Chemical Engineering laboratory (to compare calculated and experimental values), the detailed calculations of the enthalpies using heat capacity correlations are not essential. In these courses it is preferable to obtain the pure component and mixture enthalpy values at the feed and the final temperatures from an available data base such as "Aspen Properties". In such case the problem solving process proceeds according to the flow diagram in Figure 3. The model equations (which should include only the material balance equations) are entered into Polymath, as shown in

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Figure 9. Selection of the "Export to Excel" or a mouse click on the Excel icon exports the complete problem definition to a worksheet in Excel. The resulting Excel worksheet is shown in Figure 10. This equation set can be copied to any other location within the worksheet because variable cell addressed are used.

The energy balance requires enthalpy calculations for the natural gas and air fed into the burner at the initial temperature and the combustion gases at the AFT**.** These calculations can be made with enthalpies that can be accessed with the Aspen Properties Add-In for Excel. This first requires that the system of components be entered into the Aspen Properties program which is part of the Aspen Engineering Suite™. The Excel spreadsheet can then be linked to Aspen Properties to obtain the enthalpy values. This can be done as entered in the upper left of the worksheet containing the equation set as shown in Figure 11. 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, for example, 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 shown in Figure 10 (but now displaced to another location in the worksheet), and they are put in rows 9 and 12 of the spreadsheet, respectively. In rows 10 and 13 the number of moles are converted to mole fractions. In the cells B11 and B14 the molar enthalpies are calculated using the "MixtureProperty" function and in cells C11 and C14 the molar enthalpy values are multiplied by the total number of moles to obtain total enthalpy values (H_0 and H_f, repectively). In cell B15 an initial estimate for the AFT is entered, while in cell B16 the enthalpy balance equation: $f(AFT) = H_f - H_0$ is introduced. The Goal Seek utility of Excel can then be used to calculate *AFT* for one set of parameter values.

4. Using the Secant Method to Solve the Enthalpy Balance Equation

When the problem is assigned in a "Numerical Methods" course, it may be useful to require the students to program a numerical solution algorithm instead of using Goal Seek. The secant method converges very rapidly to the solution of this problem as is summarized in Figure 12.

If a numerical algorithm is used to solve the problem, the "Two Input Data Table" utility of Excel can be used to obtain the solution for all the parameter values that are specified in the problem statement. Figure 13 shows the results for some of the parameter values. When the Data Table utility is used, the parameter (*x* and *y)* values are linked, one set at a time, to the corresponding cells in the model equations. As the secant iterative method is applied, the H_f values are updated by Aspen Properties according to the current AFT values. The formula which puts the final *AFT* value into the Table is: =IF(D24<0.1,B24,"No Convergence"). The logic here is that the solution is accepted if the difference between two consecutive values of *AFT* is less

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than 0.1 otherwise the message "No Convergence" is shown. It should be pointed out that four iterations of the secant method were sufficient for convergence in all the cases tested.

5. Using the Sample Problem as Assignment in Various Courses

Table 1 summarizes the implementation details of the problem solving process for the sample problem in four core chemical engineering courses.

The emphasis on the "Stoichiometry" course is usually placed on the preparation of the mathematical model using the material and energy balance equations, a critical analysis of the results, and proper documentation of the solution. Consequently the mathematical model should be prepared by the student in detail. Aspen Properties can be used for retrieving the enthalpy values, while Polymath and Excel's Goal Seek are used to solve the problem. The Analysis of Results and Documentation steps (not shown in Table 1) are usually expected from students in all their assignments.

In the "Thermodynamics" course, it is important to emphasize the calculation of the enthalpy change for a process involving combustion. This involves the "Physical Properties" step which requires the collection of the necessary data from available tables, or databases such as Aspen Properties. The "Analysis of the Results" step in this example also involves a comparison of the AFT values for various compositions.

In a "Numerical Methods" course, the emphasis is on the performance of the numerical algorithm used to solve the problem; thus, the step of "Solution Algorithm" must be carried out in detail. There are, of course, several additional methods for solving a nonlinear equation (such as the bisection method and the Newton-Raphson method when the derivative is calculated by forward difference) than can be used and compared by solving the sample problem. The use of such realistic problems in a "Numerical Methods" course is very important in order to increase the motivation of the students to study material not directly related to chemical engineering.

In the “Chemical Engineering Laboratory”, the laboratory report typically includes a simulation of a laboratory experiment where the emphasis is on comparing measured and calculated values and discussing the adequacy or potential discrepancies of the results. In such a use only the "Analysis of the Results" and the "Documentation" steps must be carried out in detail, the remainder of the steps may optionally be assigned to be included with the laboratory report.

The easy access to physical property data for a large number of compounds, via Aspen Properties, makes it very easy to prepare many variations of the same problem, if different versions are needed for exams or homework assignments. For the sample problem presented here, for example, the natural gas can be replaced by various liquid or gaseous fuels to create different versions of the problem.

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Conclusions

Direct access to physical property data considerably reduces the effort required to prepare realistic problem assignments. When combined with the availability of user friendly numerical software packages, this gives the instructor complete control over the level of detail in which the various steps of the problem solving process should be carried out.

The availability of reliable and consistent property data enables instructors to replace artificial problems, dealing with assumed and simplified physical properties, with realistic problems dealing with real compounds. Furthermore, many different versions of the same problem can be prepared, if needed for exams and homework assignments, with minimal effort.

Real problems can be assigned routinely, as several steps of the problem solving process can be carried out very fast with the computer based tools provided. This allows the student to concentrates efforts on the steps that are most beneficial for the particular course that is being studied. This type of problem solving also mimics current industrial practice.

The proposed approach may be introduced as early as in the first CHE course, and can enable more concentrated focus on the problem formulation and solution with accurate physical property data, all within the spreadsheet environment. This may very well represent the next paradigm shift in Chemical Engineering education.

Bibliography

(1) Cutlip, M. B. and M. Shacham, *Problem Solving in Chemical Engineering with Numerical Methods*, Prentice Hall, Upper Saddle River, NJ, 1998.
(2) Fogler H. S., "An Appetizing Structure of Chemical Reaction Engineering for Undergraduates", *Chem. Eng. Ed*., **27**(2), 110(1993).
(3) Sandall, O. C., "Theoretical Maximum Flame Temperature", pp. 166-179 in Henley, E. J. (Ed). "Computer Programs for Chemical Engineering Education – Stoichiometry", CACHE Corp., Houston, Tx. (1972).

Biography of the Authors

MICHAEL B. CUTLIP is professor emeritus of the Chemical Engineering Dept. at the University of Connecticut and has served as department head and director of the university's Honors Program. He has B. Ch. E. and M. S. degrees from Ohio State and a Ph. D. from the University of Colorado. His current interests include software for engineering problem solving and educational delivery of coursework by the Internet.

MORDECHAI SHACHAM is professor and a former chair of the Department of Chemical Engineering at the Ben-Gurion University of the Negev in Israel where he has been since 1974. He received his BSc and DSc degrees from the Technion, Israel Institute of Technology. His research interest includes analysis, modeling and regression of data, applied numerical method and prediction and consistency analysis of physical properties.

MICHAEL ELLY holds B. Sc. and MBA degrees from the Ben-Gurion University of the Negev. As a part of his graduation work he developed a software application for calculating Thermodynamic Vapor Liquid Equilibrium models for which he received the Dean's Prize of Excellence. He joined Intel Corporation in 1996, serving several IT positions in Israel and in the US. Currently he works at Intel in Oregon as a Senior Automation Engineer.

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Appendix A

Calculation of Adiabatic Flame Temperature

When natural gas is burned with air, the maximum temperature that can be reached (theoretically) is the adiabatic flame temperature (AFT). This temperature depends mainly on the composition of the natural gas and the amount of air used in the burner. In this exercise the AFT's of natural gas of various compositions with different air to gas ratios are to be calculated. Natural gas consists mainly of methane, ethane, and nitrogen. The stoichiometric equations of the combustion are:

$$\begin{aligned} CH_4 + 2O_2 &\rightarrow CO_2 + 2H_2O \\ C_2H_6 + \frac{7}{2}O_2 &\rightarrow 2CO_2 + 3H_2O \end{aligned} \qquad (1)$$

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 . Thus $z = 1 - y - 0.02$.

(a) Calculate the AFT for n =7 mole fractions of methane divided equally in the region $y_{min} = 0.65$ and $y_{max} = 0.95$ (thus $y_i = y_{min} + (i\text{-}1)\,\Delta y.$, where $\Delta y. = (y_{max} - y_{min})/(n - 1)$). The calculations should be carried out for m =11 values of x, divided equally between $x_{min} = 0.5$ to $x_{max} = 2.0$.

(b) Present the results in tabular form, ascending values of y in different rows ascending values of x in different columns.

(c) Prepare a graph of AFT versus molar ratio of methane (on the x axis) and actual to theoretical molar air-to-fuel ratio (parameter).

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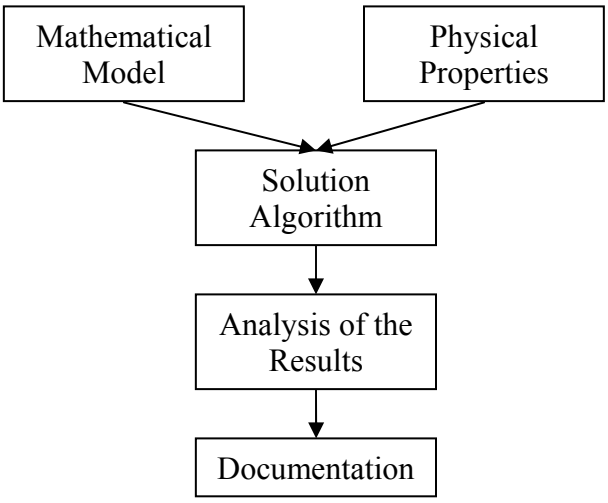

Figure 1. Problem Solving Process in Chemical Engineering

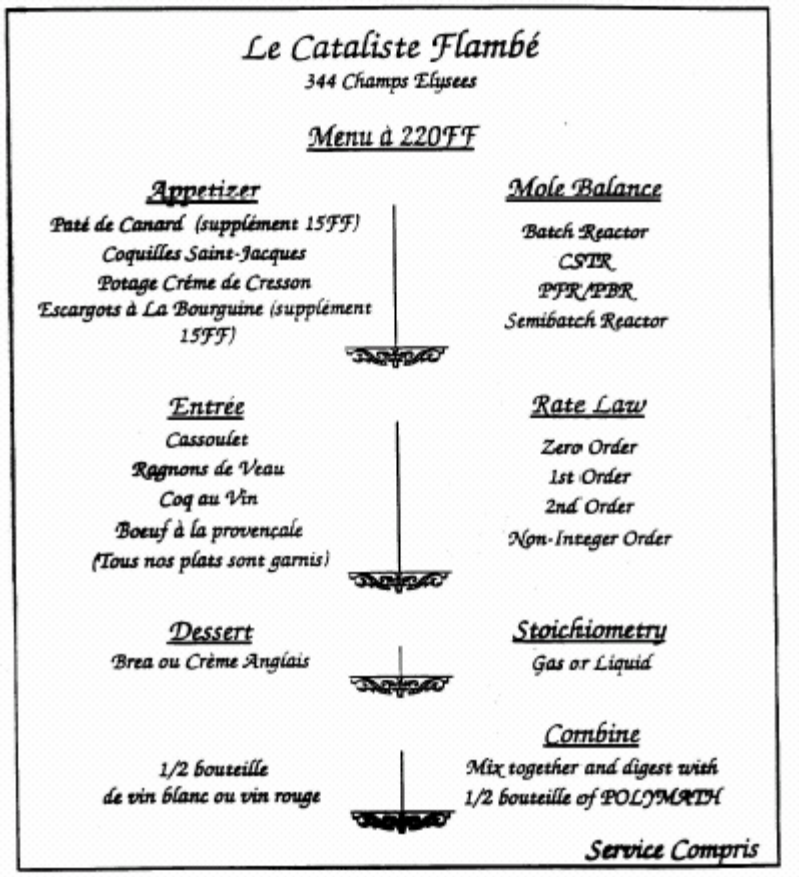

Figure 2. "French Menu" of Problem Solving in Chemical Reaction Engineering (Fogler[2]).

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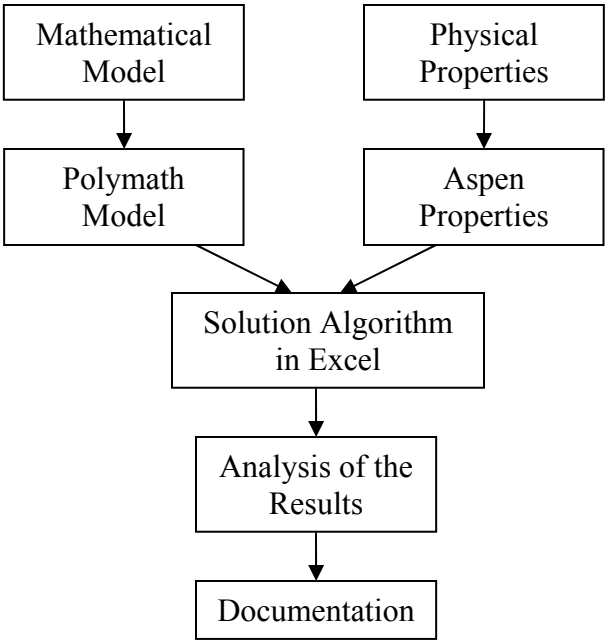

Figure 3. Problem Solving with a Combination of Software Packages

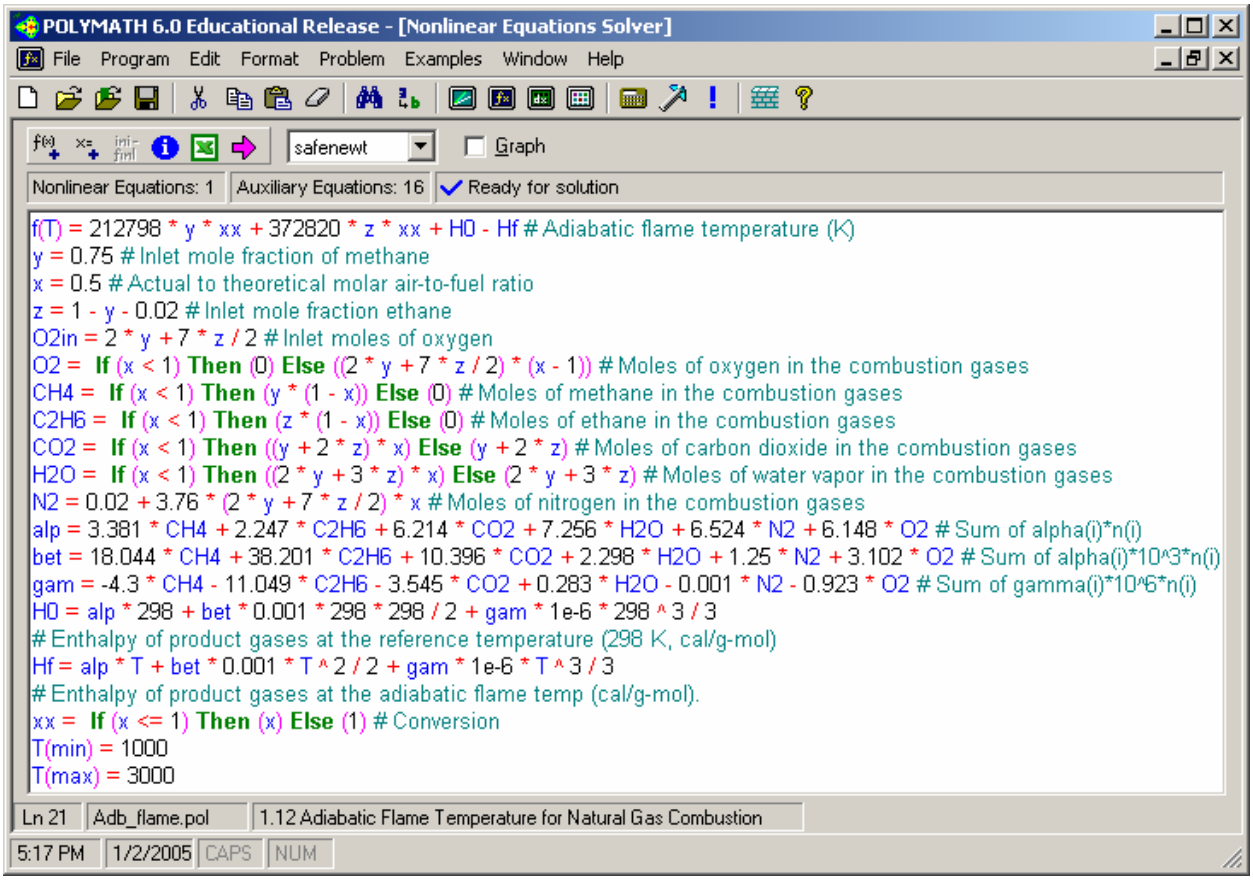

Figure 4. Polymath Editing Display with Sample Problem

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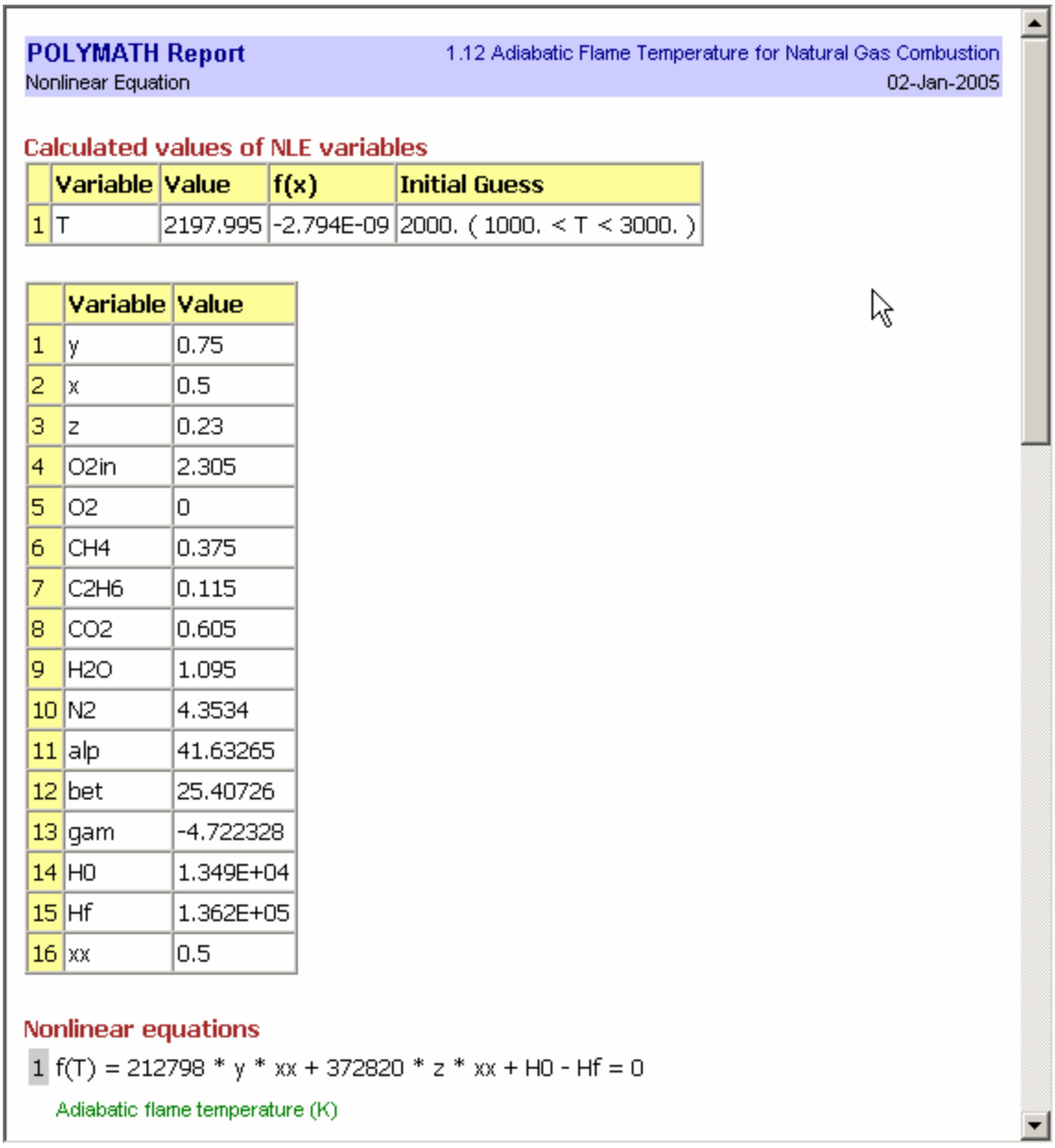

POLYMATH Report 1.12 Adiabatic Flame Temperature for Natural Gas Combustion
Nonlinear Equation 02-Jan-2005

Calculated values of NLE variables

	Variable	Value	f(x)	Initial Guess
1	T	2197.995	-2.794E-09	2000. (1000. < T < 3000.)

	Variable	Value
1	y	0.75
2	x	0.5
3	z	0.23
4	O2in	2.305
5	O2	0
6	CH4	0.375
7	C2H6	0.115
8	CO2	0.605
9	H2O	1.095
10	N2	4.3534
11	alp	41.63265
12	bet	25.40726
13	gam	-4.722328
14	H0	1.349E+04
15	Hf	1.362E+05
16	xx	0.5

Nonlinear equations

1 f(T) = 212798 * y * xx + 372820 * z * xx + H0 - Hf = 0

Adiabatic flame temperature (K)

Figure 5. Polymath Solution Report for One Case (Partial View)

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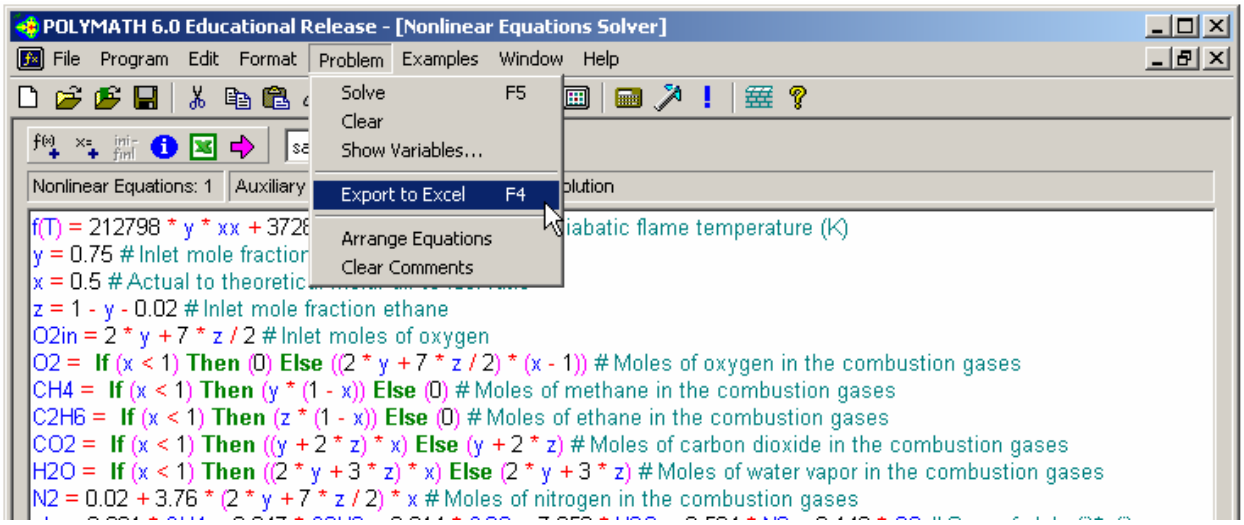

Figure 6. Polymath Editing Display for the Sample Problem with "Export to Excel Option".

	A	B	C	D	E	F
1	**POLYMATH NLE Migration Document**					
2		Variabl	Value		***Polymath Equation***	***Comments***
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 * 1*	
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 7. Excel Worksheet with Exported Problem from Polymath

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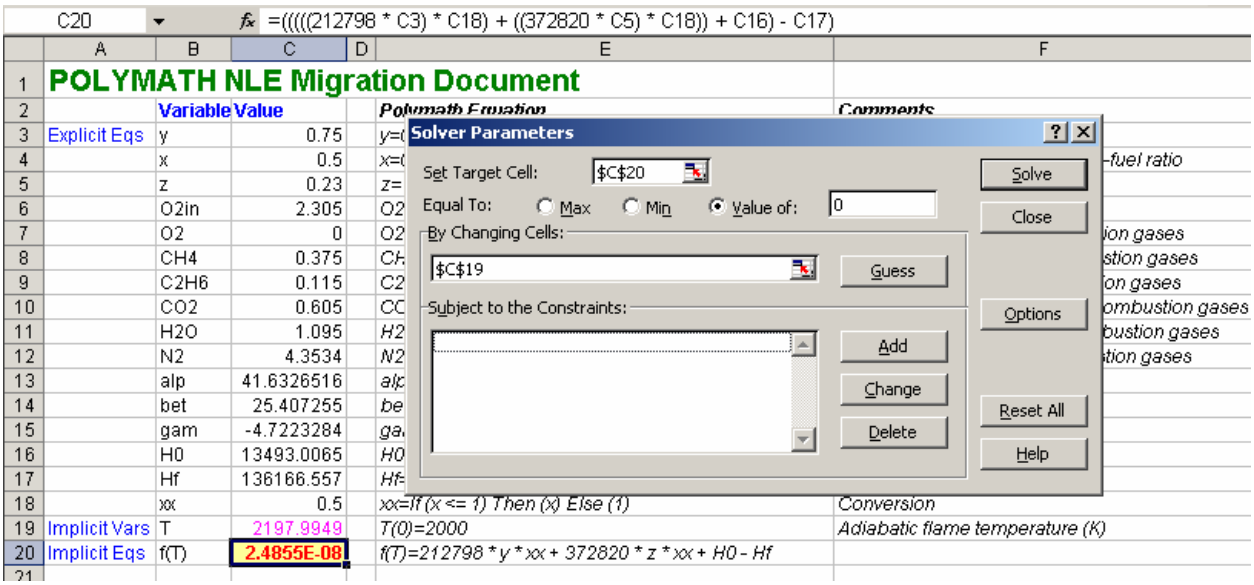

Figure 8. Use of Solver with Excel to Solve for AFT

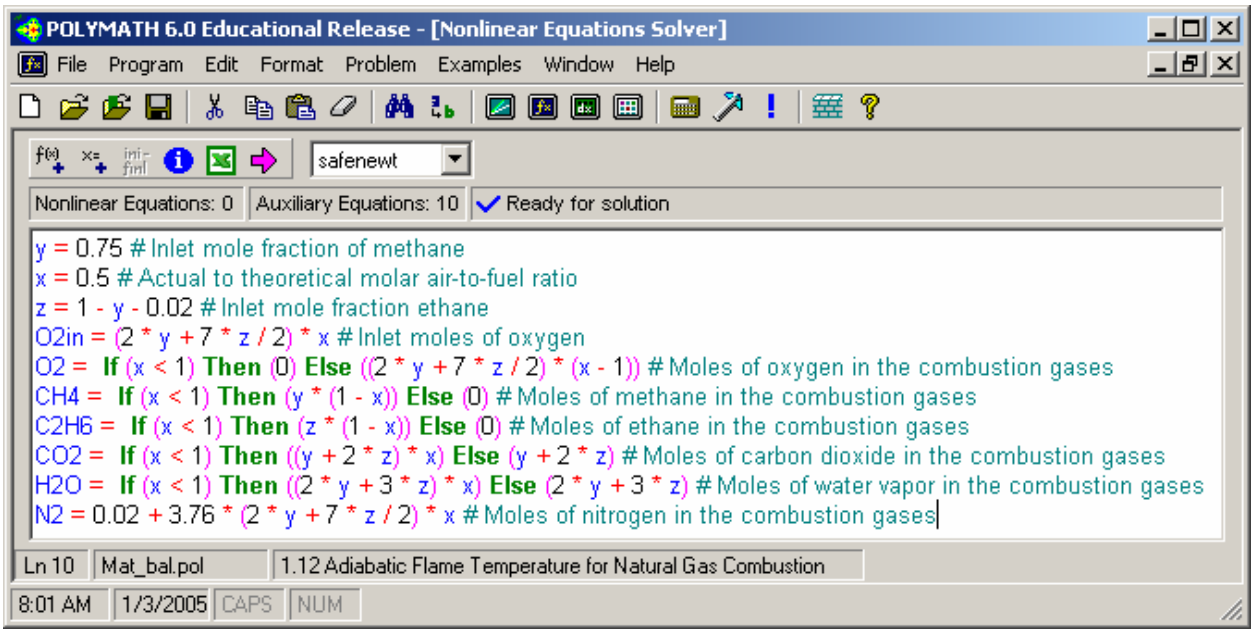

Figure 9. Polymath Program for Essential Material Balance Equations

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	A	B	C	D	E	F
1	**POLYMATH NLE Migration Document**					
2		**Variable**	**Value**		***Polymath Equation***	***Comments***
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	1.1525		*O2in=(2 * y + 7 * z / 2) * x*	*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 + 3 * z)*	*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						

Figure 10. Excel Worksheet Exported from Polymath for Essential Material Balance Equations

B14 fx =MixtureProperty(B8:G8,B13:G13,A14,B15,K5,"V")

	A	B	C	D	E	F	G
1							
2	**Computation of Adiabatic Flame Temperature**						
3							
4	**C:\Program Files\AspenTech\Aspen Properties 12.1\Engine\xeq\adb_flame.aprbkp**						
5							
6	**Global Units Set: Metrics**						
7							
8		**METHA-01**	**ETHAN-01**	**CARBO-01**	**WATER**	**OXYGE-01**	**NITRO-01**
9	**Moles in**	**0.7500**	**0.2300**	**0**	**0**	**1.1525**	**4.3534**
10	**Mole fraction**	**0.1156**	**0.0355**	**0**	**0**	**0.1777**	**0.6712**
11	**enthalpy**	**-2770.2045**	**-17967.2694**				
12	**Moles out**	**0.3750**	**0.1150**	**0.605**	**1.095**	**0**	**4.3534**
13	**Mole fraction**	**0.0573**	**0.0176**	**0.0925**	**0.1673**	**0.0000**	**0.6653**
14	**enthalpy**	**-2745.8613**	**-17967.2689**				
15	**AFT**	**1774.6627**					
16	**f(AFT)**	**0.0005**					

Figure 11. Aspen Properties Link within Excel

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C14 =SUM(B12:G12)*B14

	A	B	C	D	E	F	G
1	C:\Program Files\AspenTech\Aspen Properties 12.1\Engine\xeq\adb_flame.aprbkp						
2							
3							
4	Global Units Set:	Metrics					
5							
6							
7							
8		METHA-01	ETHAN-01	CARBO-01	WATER	OXYGE-01	NITRO-01
9	Moles in	0.75	0.23	0	0	1.1525	4.3534
10		0.115635455	0.03546154	0	0	0.17769315	0.67120986
11	enthalpy	-2770.2045	-17967.2694				
12	Moles out	0.375	0.115	0.605	1.095	0	4.3534
13	Mole fraction	0.057309656	0.017574961	0.09245958	0.1673442	0	0.66531161
14	enthalpy	-2745.861371	-17967.2693				
15							
16							
17							
18	Iteration No.	Tf	f(Tf)	err			
19	0	1000	54328.49316				
20	1	3000	-91804.6424	2000			
21	2	1743.547902	2263.193889	1256.4521			
22	3	1773.777094	64.48129075	30.2291923			
23	4	1774.66362	-0.07025938	0.88652666			
24	5	1774.662656	2.15114E-06	0.00096492			

Figure 12. Aspen Properties Link within Excel Showing AFT Iteration Results

29	x\y	y=0.65	y=0.7	y=0.75	y=0.8	y=0.85	y=0.9	y=0.95
30	1774.662656	0.65	0.7	0.75	0.8	0.85	0.9	0.95
31	0.5	1781.636326	1778.253805	1774.66266	1770.8429	1766.77208	1762.42444	1757.771
32	0.65	1904.170307	1900.794933	1897.20936	1893.3933	1889.323769	1884.97463	1880.316
33	0.8	1992.247618	1988.923222	1985.3902	1981.6283	1977.614412	1973.32244	1968.722
34	0.95	2058.674756	2055.415966	2051.9514	2048.2609	2044.321694	2040.10766	2035.589
35	1.1	1937.179763	1934.279061	1931.19435	1927.9075	1924.398067	1920.64254	1916.614
36	1.25	1760.537059	1758.030285	1755.36392	1752.5222	1749.487321	1746.23878	1742.753
37	1.4	1614.687732	1612.482614	1610.13671	1607.6361	1604.964922	1602.10514	1599.036
38	1.55	1492.129204	1490.16147	1488.06781	1485.8357	1483.451045	1480.89753	1478.157
39	1.7	1387.622706	1385.846085	1383.95555	1381.9398	1379.785877	1377.47917	1375.003
40	1.85	1297.398262	1295.7785	1294.05471	1292.2165	1290.252182	1288.14822	1285.889
41	2	1218.672862	1217.183988	1215.59936	1213.9094	1212.103322	1210.16865	1208.091

Figure 13. AFT Values for Different Methane–Ethane (*y*) and Natural Gas–Air (x) Ratios

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Table 1. Implementation of the Problem Solving Stages for the Sample Problem in Various Courses.

Course	Solution Process Stage	Mathematical Model	Physical Properties	Solution Algorithm
Stoichiometry		In detail	Aspen Properties	Polymath and Excel Goal Seek
Thermodynamics		In detail	In detail	Polymath and Excel Goal Seek
Numerical Methods		In detail, or provided by the instructor	Aspen Properties	Polymath and a Numerical Technique in Excel
Chemical Engineering Laboratory		In detail, or provided by the instructor	Aspen Properties	Polymath and Excel Goal Seek

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