Efficient Solution of Numerical Problems within Polymath and Excel

MB Cutlip, Dept. of Chemical Engineering, University of Connecticut, Storrs, CT 06269, USA (e-mail: michael.cutlip@uconn.edu)

M Shacham, Dept. of Chemical Engineering, Ben-Gurion University of the Negev, Beer-Sheva 84105, Israel (e-mail: shacham@bgumail.bgu.ac.il)

M Elly, Intel Corporation, Qiryat Gat, Israel (e-mail: michael.a.elly@intel.com)

Introduction

Chemical Engineering educators are continually challenged with the need to enable students to solve complex problems that require numerical methods. We have developed and extended the user-friendly Polymath[1] package for this purpose since 1984. The CACHE Corporation[2] has been very supportive of this effort and has made inexpensive site licenses of Polymath available to the world-wide academic community since 1990. The software runs on all personal computers with Windows™ operating systems. Current capabilities of Polymath include:

- Simultaneous Linear Equations
- Simultaneous Nonlinear Algebraic Equations
- Simultaneous Ordinary Differential Equations
- Data Analysis and Regression - linear, multiple linear, and nonlinear regressions with extensive statistics plus polynomial and spline fitting with interpolation and graphing capabilities

This software is currently provided with five textbooks and has been the referenced calculational tool for many educational publications. Users recognize that this package is perhaps the easiest-to-use software that is available for educational use as it enables very straightforward input in mathematical equation format and requires a minimal learning curve.

Exporting Problems from Polymath to Excel

The latest Polymath release in December of 2004 has many new features including the novel capability of automatically exporting a complete problem from Polymath directly into Excel[3] with one keypress. The created spreadsheet can then be used to solve the problem and problem variations independently of Polymath. The export capability includes conversion all of the

[1] POLYMATH is copyrighted by M. Shacham, M. B. Cutlip and M. Elly (http://www.polymath-software.com).
[2] Computer Aids for Chemical Engineering Corporation (http://www.cache.org).
[3] Excel is a trademark of Microsoft Corporation (http://www.microsoft.com).

intrinsic functions and logical functionality found within Polymath. Within Excel, the "Solver" Add-In is used for nonlinear equations and nonlinear regressions. The LINEST functionality in Excel is used for linear regressions. For differential equations, we have created an Ode_Solver Add-In for Excel that numerically integrates simultaneous ordinary differential equations.

This software provides educators and their students with problem solving capabilities for a numerical computation package (Polymath) and also a spreadsheet package (Excel). Thus students become familiar with both of these environments. Most importantly, this enables more complex and realistic problems to be posed and easily solved in chemical engineering education.

Incorporation of Physical Property Data in Excel

A recent addition to the capabilities within Excel is the availability of the Aspen Properties™ Add-In from AspenTech[4] that gives users access to advanced physical property data during problem solving within Excel. This capability of calling upon realistic physical properties during student problem solving may well represent an important new paradigm in Chemical Engineering Education.

An Example Problem - Cocurrent Operation of a Double Pipe Heat Exchanger

The usefulness of Polymath, Excel, and Aspen Properties will be illustrated with the following problem involving a double pipe heat exchanger from Cutlip, M. B. and M. Shacham (1).

Consider a concurrent double pipe heat exchanger with cooling water in the shell side and benzene in the tube side. The cooling water is available at 65 °F and has a flow that is three times that of the benzene. The inlet benzene temperature is 150 °F. The configuration of the heat exchanger is given below in Figure 1.

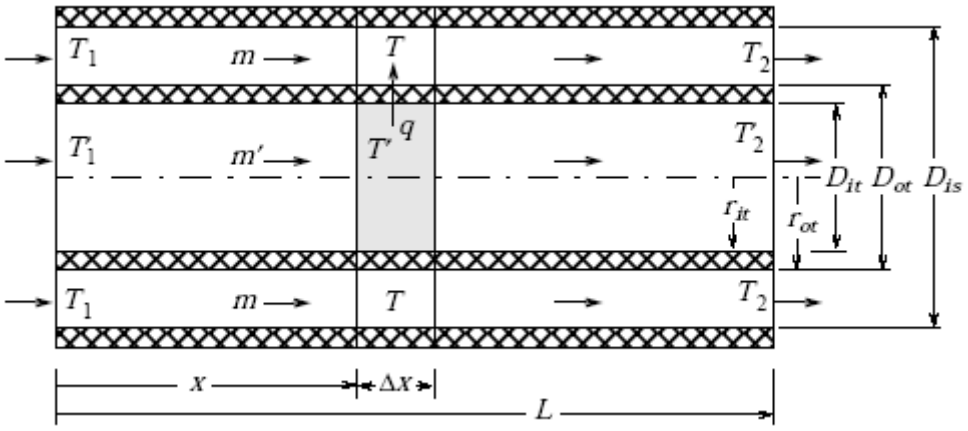


Figure 1 – Double Pipe Heat Exchanger

[4] Aspen Properties is a registered product of AspenTech (http://www.aspentech.com).

Equation (1) represents the local heat transfer coefficient where the exponent n = 0.4 for heating and 0.3 for cooling.

$$\frac{hD}{k} = 0.023\left(\frac{Dv\rho}{\mu}\right)^{0.8}\left(\frac{C_p\mu}{k}\right)^{n} \tag{1}$$

The local overall heat transfer coefficient based on the inside area can be calculated from Geankoplis (2)

$$U_i = \frac{1}{1/h_i + ((r_{ot} - r_{it})D_{it})/(k_t D_{tlm}) + D_{it}/(D_{ot}h_o)} \tag{2}$$

where t represents the tube wall material and dimensions. The D_{tlm} term is the log mean diameter (or area) for the tube wall.

A differential energy balance on the benzene streawm in the tube yields the following differential equation where the prime indicates that the benzene properties are to be evaluated at the local temperature of the benzene.

$$\frac{d}{dx}(T') = -\frac{U_i(\pi D_i)(T' - T)}{m' C_p'} \tag{3}$$

Similarly for the insulated shell side, a differential energy balance yields the following differential equation where the physical properties of water are to be evaluated at the local temperature of the water.

$$\frac{dT}{dx} = \frac{U_i(\pi D_i)(T' - T)}{mC_p} \tag{4}$$

Solution of Sample Problem

This sample problem will be solved in three ways:

1) The Polymath program will be used to solve the problem for the case where the physical properties are assumed to be constant at the inlet temperatures to the heat exchanger.
2) The exported problem from Polymath to Excel will be solved completely within Excel using the Polymath Ode_Solver Add-In.
3) The problem in Excel will be solved with the physical properties provided by the Aspen Properties Excel Add-In, and the solution of the differential equations will use the Polymath Ode_Solver Add-In.

Polymath Program Solution – Constant Physical Properties

The entry of this problem into the Polymath editor for the Differential Equations Solver is shown in Figure 1. Note that the equations can be entered in any order as Polymath will order the equations before solution. The equations with the comments contain the physical property variables that are entered as constants in this program at the initial temperatures for simplicity.

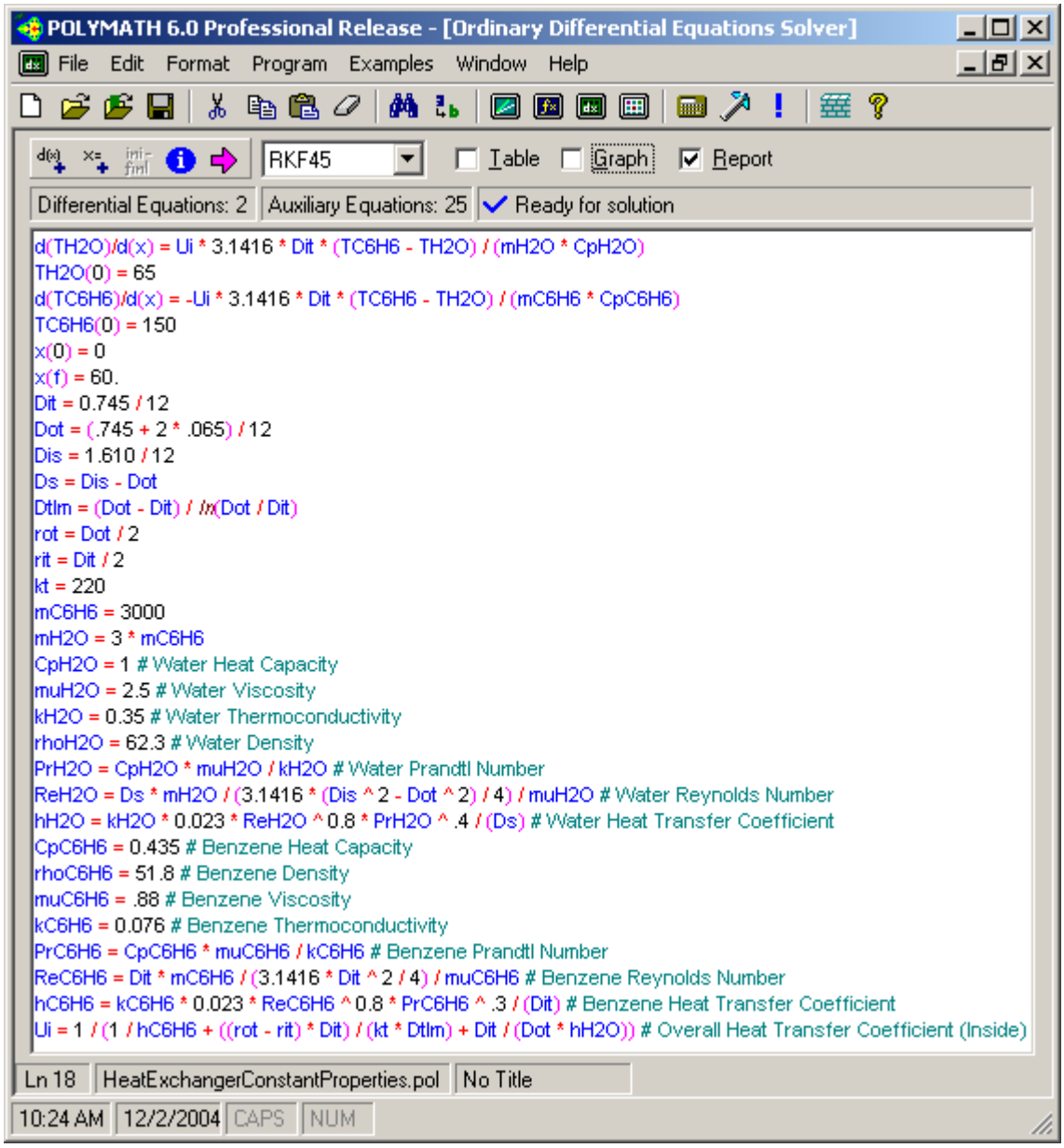
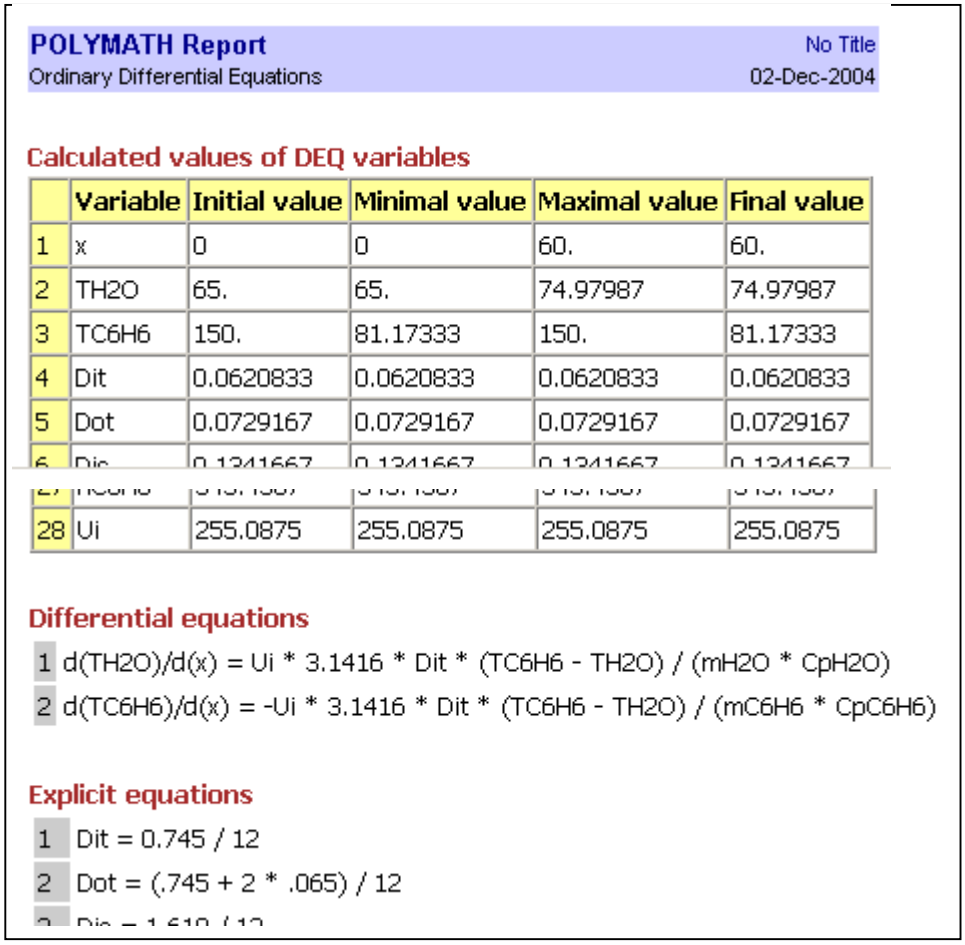


Figure 1 – Polymath Editing Display for Sample Problem (Differential Equation Sover)

The solution of this problem with a single mouse click on the purple arrow icon in Polymath yields a 'Report' in which general information regarding the solution is provided. Many other options are available including graphical and tabular output. Portions of the 'Report' are reproduced in Figure 2. Note that the initial value, minimal value, maximal value, and final value of all the problem variables are summarized in this 'Report'. In addition, the various differential equations and the explicit equations are also given. The complete ordered equation set with the comments is also provided (not shown in the figure).



POLYMATH Report No Title
Ordinary Differential Equations 02-Dec-2004

Calculated values of DEQ variables

	Variable	Initial value	Minimal value	Maximal value	Final value
1	x	0	0	60.	60.
2	TH2O	65.	65.	74.97987	74.97987
3	TC6H6	150.	81.17333	150.	81.17333
4	Dit	0.0620833	0.0620833	0.0620833	0.0620833
5	Dot	0.0729167	0.0729167	0.0729167	0.0729167
6	Dic	0.1241667	0.1241667	0.1241667	0.1241667
28	Ui	255.0875	255.0875	255.0875	255.0875

Differential equations

1 d(TH2O)/d(x) = Ui * 3.1416 * Dit * (TC6H6 - TH2O) / (mH2O * CpH2O)
2 d(TC6H6)/d(x) = -Ui * 3.1416 * Dit * (TC6H6 - TH2O) / (mC6H6 * CpC6H6)

Explicit equations

1 Dit = 0.745 / 12
2 Dot = (.745 + 2 * .065) / 12

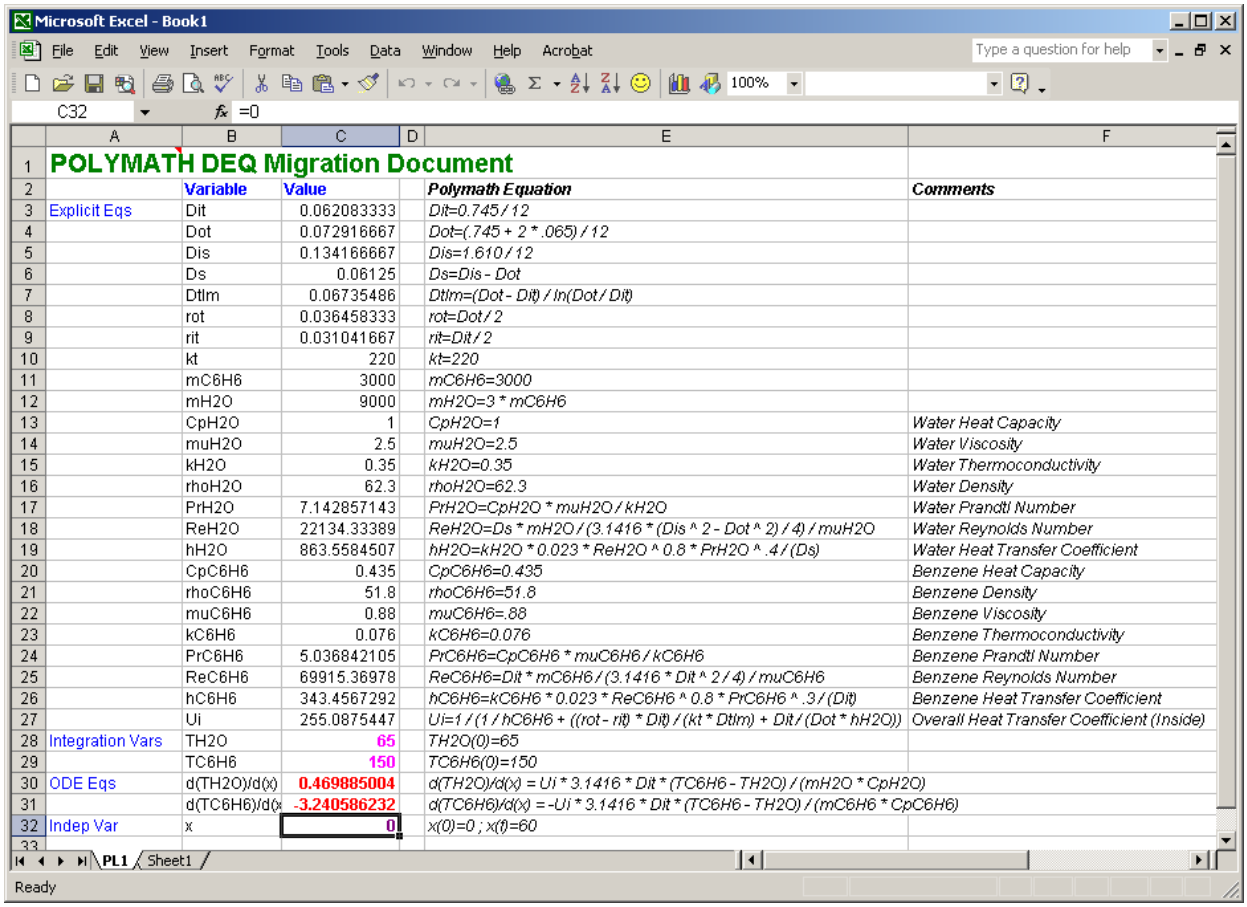
Figure 2 – Partial Screen Display of Polymath Report

Polymath Export to Excel

This problem can be exported from the Polymath Differential Equations Editor to Excel with a single keypress. During this automatic export process, all the intrinsic functions and logical variables are converted to their equivalents in the code for the spreadsheet. Once any problem has been exported to Excel, the numerical solutions can be completely accomplished within Excel. The Excel "Solver" can be used for solving nonlinear algebraic equations. Regression problems utilize the Excel “LINEST” function or “Solver”. For systems of ODE’s (ordinary differential equations), the Polymath Ode_Solver Add-In for Excel must be used.

The resulting Excel worksheet is shown in Figure 3. In the Excel 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 d(TH2O)/d(x) for example is:

d(TH2O)/d(x) = ((((C27 * 3.1416) * C3) * (C29 - C28)) / (C12 * C13))



Microsoft Excel - Book1

File Edit View Insert Format Tools Data Window Help Acrobat — Type a question for help

C32 =0

	A	B	C	D	E	F
1	**POLYMATH DEQ Migration Document**					
2		**Variable**	**Value**		***Polymath Equation***	***Comments***
3	Explicit Eqs	Dit	0.062083333		*Dit=0.745 / 12*	
4		Dot	0.072916667		*Dot=(.745 + 2 * .065) / 12*	
5		Dis	0.134166667		*Dis=1.610 / 12*	
6		Ds	0.06125		*Ds=Dis - Dot*	
7		Dtlm	0.06735486		*Dtlm=(Dot - Dit) / ln(Dot / Dit)*	
8		rot	0.036458333		*rot=Dot / 2*	
9		rit	0.031041667		*rit=Dit / 2*	
10		kt	220		*kt=220*	
11		mC6H6	3000		*mC6H6=3000*	
12		mH2O	9000		*mH2O=3 * mC6H6*	
13		CpH2O	1		*CpH2O=1*	*Water Heat Capacity*
14		muH2O	2.5		*muH2O=2.5*	*Water Viscosity*
15		kH2O	0.35		*kH2O=0.35*	*Water Thermoconductivity*
16		rhoH2O	62.3		*rhoH2O=62.3*	*Water Density*
17		PrH2O	7.142857143		*PrH2O=CpH2O * muH2O / kH2O*	*Water Prandtl Number*
18		ReH2O	22134.33389		*ReH2O=Ds * mH2O / (3.1416 * (Dis ^ 2 - Dot ^ 2) / 4) / muH2O*	*Water Reynolds Number*
19		hH2O	863.5584507		*hH2O=kH2O * 0.023 * ReH2O ^ 0.8 * PrH2O ^ .4 / (Ds)*	*Water Heat Transfer Coefficient*
20		CpC6H6	0.435		*CpC6H6=0.435*	*Benzene Heat Capacity*
21		rhoC6H6	51.8		*rhoC6H6=51.8*	*Benzene Density*
22		muC6H6	0.88		*muC6H6=.88*	*Benzene Viscosity*
23		kC6H6	0.076		*kC6H6=0.076*	*Benzene Thermoconductivity*
24		PrC6H6	5.036842105		*PrC6H6=CpC6H6 * muC6H6 / kC6H6*	*Benzene Prandtl Number*
25		ReC6H6	69915.36978		*ReC6H6=Dit * mC6H6 / (3.1416 * Dit ^ 2 / 4) / muC6H6*	*Benzene Reynolds Number*
26		hC6H6	343.4567292		*hC6H6=kC6H6 * 0.023 * ReC6H6 ^ 0.8 * PrC6H6 ^ .3 / (Dit)*	*Benzene Heat Transfer Coefficient*
27		Ui	255.0875447		*Ui=1 / (1 / hC6H6 + ((rot - rit) * Dit) / (kt * Dtlm) + Dit / (Dot * hH2O))*	*Overall Heat Transfer Coefficient (Inside)*
28	Integration Vars	TH2O	65		*TH2O(0)=65*	
29		TC6H6	150		*TC6H6(0)=150*	
30	ODE Eqs	d(TH2O)/d(x)	0.469885004		*d(TH2O)/d(x) = Ui * 3.1416 * Dit * (TC6H6 - TH2O) / (mH2O * CpH2O)*	
31		d(TC6H6)/d(x	-3.240586232		*d(TC6H6)/d(x) = -Ui * 3.1416 * Dit * (TC6H6 - TH2O) / (mC6H6 * CpC6H6)*	
32	Indep Var	x	0		*x(0)=0 ; x(f)=60*	
33						

PL1 Sheet1

Ready

Figure 3 – Exported Program from Polymath to Excel

Thus the exported problem is ready for solution within Excel.

Excel Solution – Constant Physical Properties

The Polymath Ode_Solver Add-In that has been developed to work independently within Excel. It is an Add-In just like ‘Solver” which is supplied with Excel for solving nonlinear equations. The Ode_Solver requires input of the following cell addresses and numerical values: 1) The range of the cells where the initial values of the differential equations are stored; 2) The range of the cells where the formulas of the differential equations are stored; 3) The cell where the initial value for the independent variable (time, in this case) is stored; 4) The final value of the independent variable; 5) The range of cells where formulas of additional variables for which the integration results should be stored (optional).

Solution of the differential equations is implemented by clicking on the Ode_Solver in the ‘Tools’ menu of Excel. This brings up the display shown in Figure 4 where the various input cells have been identified. Note that 101 data points have been requested for this problem which can be used for graphical presentation of the results. No other variables have been specified. The **Adv.** button allows selection of a particular integration algorithm and its parameters.

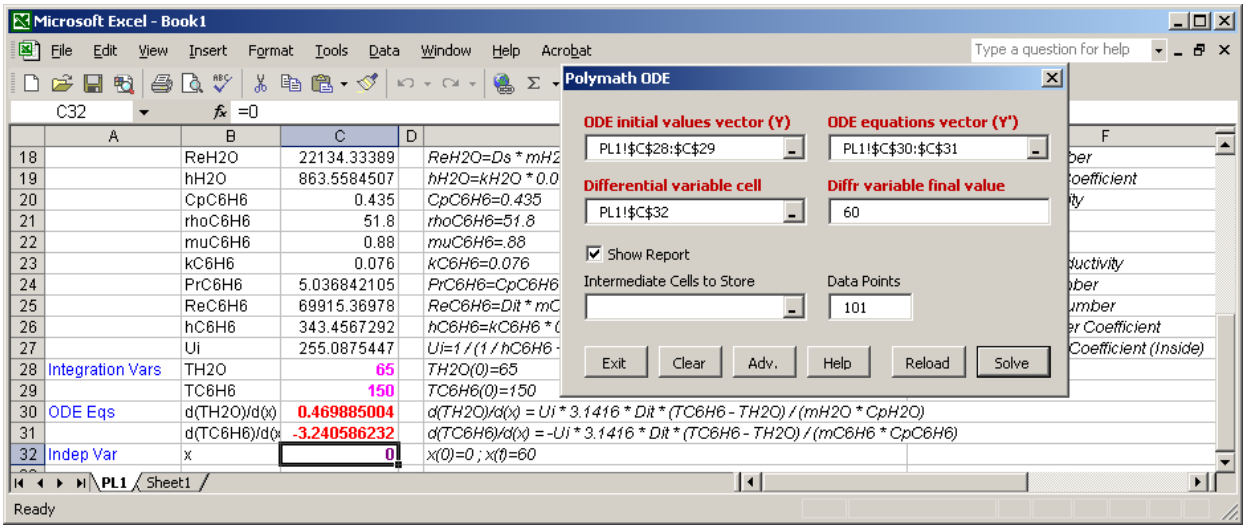
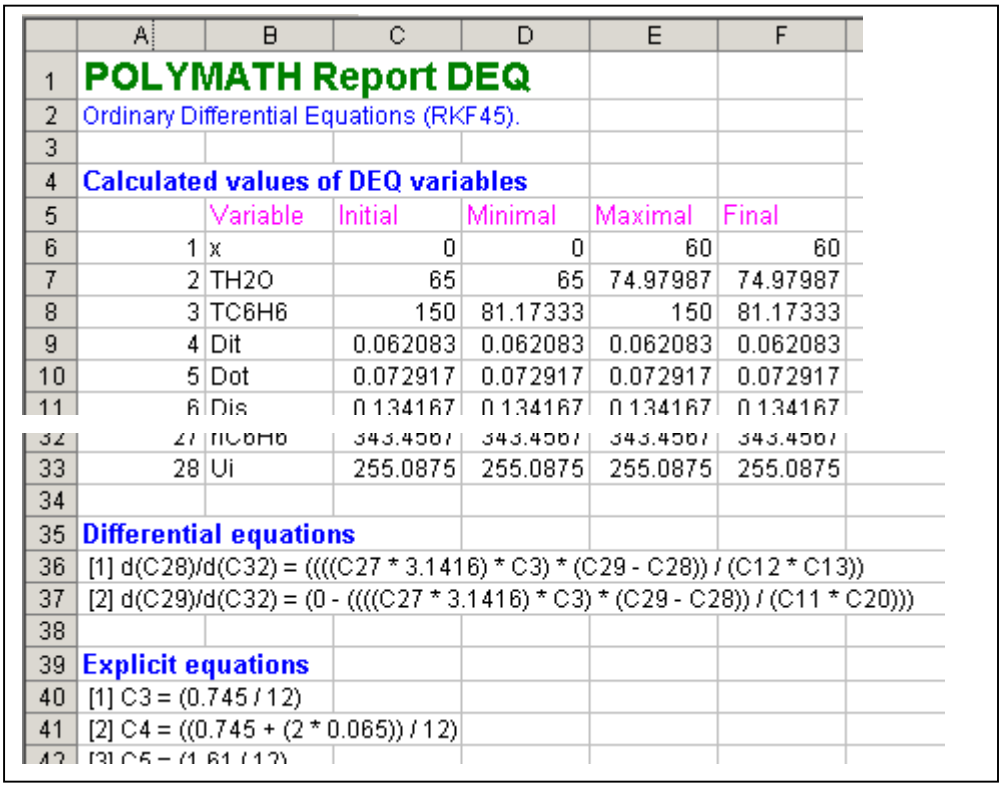


Figure 4 – Ode_Solver Input Window within Sample Problem

During the real-time solution of the differential equations within Excel, the cells with the blue titles (Integration Vars, ODE EQS, and Indep Var) in column C of Figure 3 change as the integration proceeds. A new worksheet is then created in the Excel workbook that contains a 'Report' of the problem solution. This is partly shown in Figure 5, although the table of variables is not shown but is always generated within this Excel solution 'Report'. The 'Reports' of Figure 2 (Polymath Solution) and Figure 5 (Excel Solutions) are exactly equivalent.



POLYMATH Report DEQ

Ordinary Differential Equations (RKF45).

Calculated values of DEQ variables

	Variable	Initial	Minimal	Maximal	Final
1	x	0	0	60	60
2	TH2O	65	65	74.97987	74.97987
3	TC6H6	150	81.17333	150	81.17333
4	Dit	0.062083	0.062083	0.062083	0.062083
5	Dot	0.072917	0.072917	0.072917	0.072917
6	Dis	0.134167	0.134167	0.134167	0.134167
27	mC6H6	343.4567	343.4567	343.4567	343.4567
28	Ui	255.0875	255.0875	255.0875	255.0875

Differential equations

[1] d(C28)/d(C32) = ((((C27 * 3.1416) * C3) * (C29 - C28)) / (C12 * C13))

[2] d(C29)/d(C32) = (0 - ((((C27 * 3.1416) * C3) * (C29 - C28)) / (C11 * C20)))

Explicit equations

[1] C3 = (0.745 / 12)

[2] C4 = ((0.745 + (2 * 0.065)) / 12)

Figure 5 – Partial View of Excel Spreadsheet Giving Problem Report Information

Excel Solution – Variable Physical Properties

The variation of the physical properties of the benzene and water in this sample problem can be accommodated 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 a part of the Aspen Engineering Suite. The then allows the user to setup a location within the Excel spreadsheet that can link the spreadsheet to Aspen Properties as shown in Figure 6. The Aspen file is colored purple in the spreadsheet.

	A	B	C	D
1	Cocurrent Operation of a Double Pipe Heat Exchanger			
2				
3	C:\Heat_exchange.aprbkp			
4				
5	Global Units Set: English			
6				
7		WATER	BENZE-01	
8	viscosity	1.06182393	0.373087253	
9	thermalConductivi	0.83916422	0.075791638	
10	heatCapacity	17.9766545	32.82721459	
11	density	3.46063356	0.668678142	
12	molecularWeight	18.01528	78.11364	
13	pressure	14.7		
14	temperature	65	150	

Figure 6 – Aspen Properties Link in Excel

This portion of the spreadsheet responds to changes in temperature and pressure by updating the contents of the cells that contain the physical properties data.

The physical property data can be integrated together with the problem solution by copying the exported worksheet from Polymath to Excel with the constant physical properties shown in Figure 3 to the worksheet in Figure 6. This integrated spreadsheet is presented in Figure 7. Note that some conversion factors have been entered into the cell where the physical properties are found to achieve consistency in the units. The highlighted rows in Figure 7 indicate the property variables that vary with temperature. As the value of the water temperature in cell C42 changes, then all of the properties of water change. As the value of the benzene temperature in cell C43 changes, then the properties of benzene adjust accordingly. Thus all of the other equations are updated as these temperatures change during the course of the numerical integration of the differential equations.

	A	B	C	D	E	F	G
1	Cocurrent Operation of a Double Pipe Heat Exchanger						
2							
3	C:\Heat_exchange.aprbkp						
4							
5	Global Units Set: English						
6							
7		WATER	BENZE-01				
8	viscosity	1.06182393	0.373087253				
9	thermalConductivity	0.73914296	0.075791638				
10	heatCapacity	17.9766545	32.82721459				
11	density	3.46063356	0.668678142				
12	molecularWeight	18.01528	78.11364				
13	pressure	14.7					
14							
15	POLYMATH DEQ Migration Document						
16		Variable	Value		Polymath Equation	Comments	
17	Explicit Eqs	Dit	0.062083333		Dit=0.745 / 12		
18		Dot	0.072916667		Dot=(.745 + 2 * .065) / 12		
19		Dis	0.134166667		Dis=1.610 / 12		
20		Ds	0.06125		Ds=Dis - Dot		
21		Dtlm	0.06735486		Dtlm=(Dot - Dit) / ln(Dot / Dit)		
22		rot	0.036458333		rot=Dot / 2		
23		rit	0.031041667		rit=Dit / 2		
24		kt	220		kt=220		
25		mC6H6	3000		mC6H6=3000		
26		mH2O	9000		mH2O=3 * mC6H6		
27		CpH2O	0.997855961		CpH2O=Aspen Properties	Water Heat Capacity	
28		muH2O	2.568658264		muH2O=Aspen Properties	Water Viscosity	
29		kH2O	0.739142961		kH2O=Aspen Properties	Water Thermoconductivity	
30		rhoH2O	62.34428265		rhoH2O=Aspen Properties	Water Density	
31		PrH2O	3.467733706		PrH2O=CpH2O * muH2O / kH2O	Water Prandtl Number	
32		ReH2O	21542.70013		ReH2O=Ds * mH2O / (3.1416 * (Dis ^ 2 - Dot ^ 2) / 4) / muH2O	Water Reynolds Number	
33		hH2O	1336.621964		hH2O=kH2O * 0.023 * ReH2O ^ 0.8 * PrH2O ^ .4 / (Ds)	Water Heat Transfer Coefficient	
34		CpC6H6	0.420249454		CpC6H6=Aspen Properties	Benzene Heat Capacity	
35		rhoC6H6	52.23288364		rhoC6H6=Aspen Properties	Benzene Density	
36		muC6H6	0.902535373		muC6H6=Aspen Properties	Benzene Viscosity	
37		kC6H6	0.075791638		kC6H6=Aspen Properties	Benzene Thermoconductivity	
38		PrC6H6	5.004377922		PrC6H6=CpC6H6 * muC6H6 / kC6H6	Benzene Prandtl Number	
39		ReC6H6	68169.65543		ReC6H6=Dit * mC6H6 / (3.1416 * Dit ^ 2 / 4) / muC6H6	Benzene Reynolds Number	
40		hC6H6	335.0055556		hC6H6=kC6H6 * 0.023 * ReC6H6 ^ 0.8 * PrC6H6 ^ .3 / (Dit)	Benzene Heat Transfer Coefficient	
41		Ui	274.3695259		Ui=1 / (1 / hC6H6 + ((rot - rit) * Dit) / (kt * Dtlm) + Dit / (Dot * hH2O))	Overall Heat Transfer Coefficient (Inside)	
42	Integration Vars	TH2O	65		TH2O(0)=65		
43		TC6H6	150		TC6H6(0)=150		
44	ODE Eqs	d(TH2O)/d(x)	0.506489385		d(TH2O)/d(x) = Ui * 3.1416 * Dit * (TC6H6 - TH2O) / (mH2O * CpH2O)		
45		d(TC6H6)/d(x	-3.6078818		d(TC6H6)/d(x) = -Ui * 3.1416 * Dit * (TC6H6 - TH2O) / (mC6H6 * CpC6H6)		
46	Indep Var	x	0		x(0)=0 ; x(f)=60		

Figure 7 – Integrated Aspen Properties and Polymath to Excel Spreadsheet

1	POLYMATH Report DEQ					
2	Ordinary Differential Equations (RKF45).					
3						
4	Calculated values of DEQ variables					
5		Variable	Initial	Minimal	Maximal	Final
6	1	x	0	0	60	60
7	2	TH2O	65	65	74.40232	74.40232
8	3	TC6H6	150	79.36953	150	79.36953
9						

Figure 8 - Partial Report for Excel Solution with Variable Physical Properties

It is interesting to compare the results from the solution with constant physical properties given in Figure 2 with the solution with variable physical properties given in Figure 8. The benzene outlet temperature is about 0.6 °F higher and the water outlet temperature is about 1.8 °F higher.

Conclusions

1) The Polymath package provides problem solving software on personal computers that can be widely utilized in Chemical Engineering Education. The latest version includes options for easily exporting problems to Excel for execution directly within the spreadsheet.
2) The Polymath Ode_Solver for Excel, available as an Add-In, allows the convenient solution of systems of ordinary differential equations within a spreadsheet. This will allow more advanced problem solving among both students and professional engineers as the Excel software is quite widely used.
3) Physical property data can be introduced into problem solving in Excel through the use of the Aspen Properties Add-In. This provides access to the extensive physical property data bases of the Aspen Engineering Suite.
4) The use of problem solving with convenient access to physical property data has the potential to become a new paradigm in Chemical Engineering Education. The introduction of this capability to beginning students will greatly impact the ways in which problems will be posed and solved throughout the curriculum. It will allow more realistic problems to be posed and efficiently solved throughout the educational program of chemical engineers. It has the potential to be quite valuable in their professional engineering careers.

References

1. Cutlip, M. B. and M. Shacham, *Problem Solving in Chemical Engineering with Numerical Methods*, Prentice Hall, Upper Saddle River, NJ, 1998.
2. Geankoplis, C. J., *Transport Processes and Separation Process Principles*, 4th ed., Prentice Hall, Upper Saddle River, NJ, 2003.