POLYMATH 6 Now Works with Excel© and MATLAB™

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There is considerable interest in the latest capabilities within POLYMATH© that allow direct connections to problem solving utilizing Excel and MATLAB. The following brief discussion indicates how the Excel connections work. The Spring 2006 CACHE Newsletter will focus on the MATLAB connection in which an "M" file is generated.

Information on the special site license versions of POLYMATH is available from the CACHE web site: http://www.che.utexas.edu/cache/polymath.html

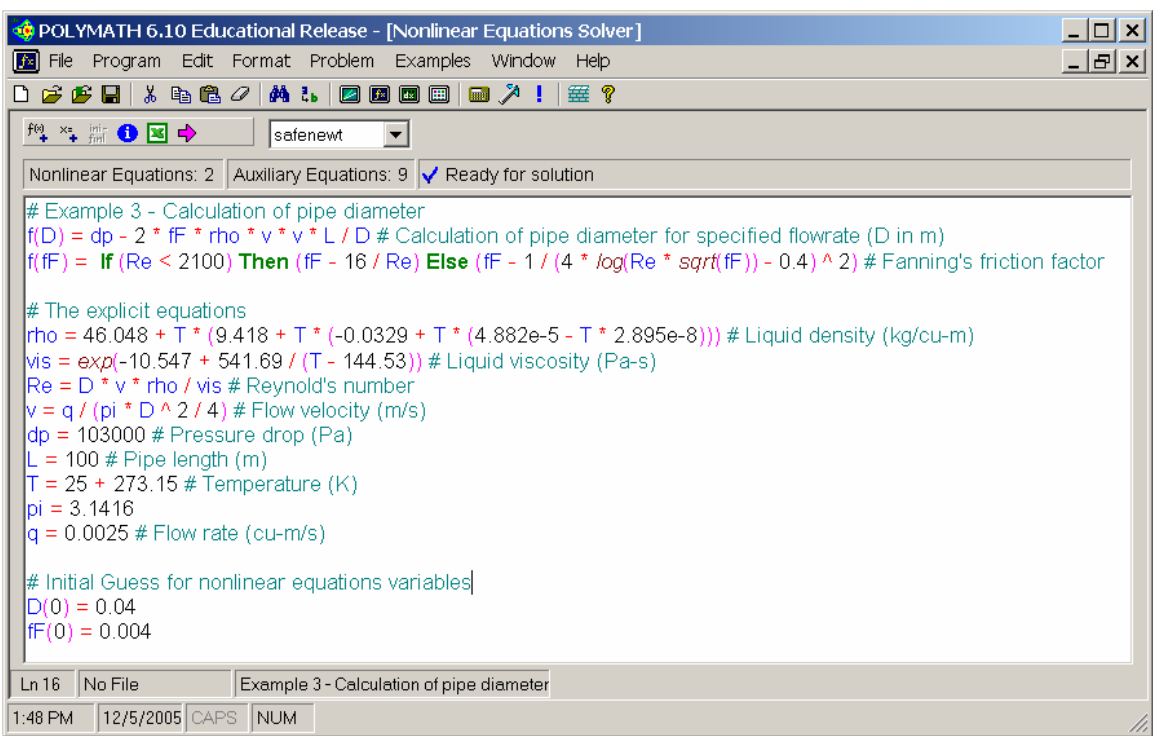
Excel Connection

Most POLYMATH programs can now be easily exported to Excel. This is accomplished by a single key press on the Excel icon from the POLYMATH program.

This export results in a direct translation of the POLYMATH program into a working Excel program and includes all intrinsic functions and logical variables. The Excel program is well documented and can be used independently of the POLYMATH program.

POLYMATH Example 3 for the Nonlinear Equation Solver

Consider Example 3 from POLYMATH 6 for the Nonlinear Equation Solver. This program is shown below.



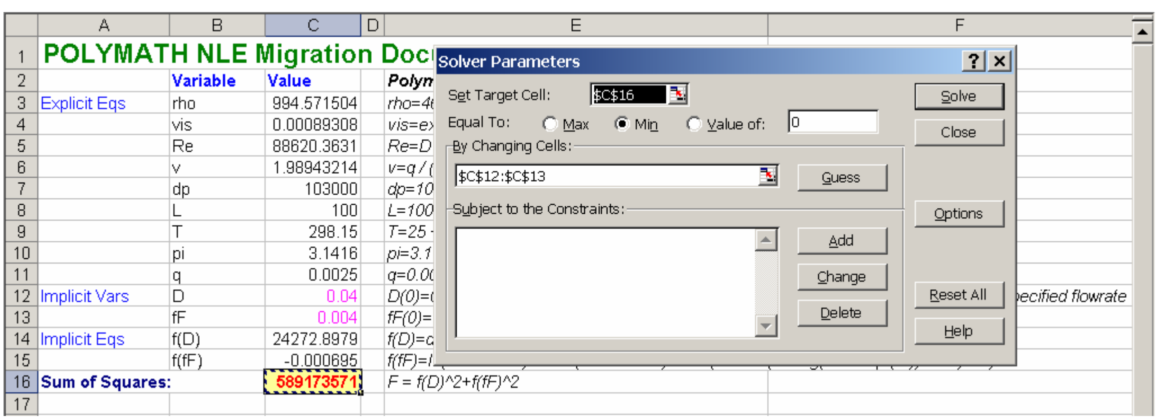
A single mouse click on the Excel icon takes this problem directly to an Excel workbook. Note that this export to Excel maintains the original problem using the same variable definitions and also presents the original POLYMATH equations and comments. The "Sum of Squares" cell is formed by summing all of the nonlinear equations.

	A	B	C	D	E	F
1	POLYMATH NLE Migration Document					
2		Variable	Value		Polymath Equation	Comments
3	Explicit Eqs	rho	994.571504		rho=46.048 + T * (9.418 + T * (-0.0329 + T * (4.882e	Liquid density (kg/cu-m)
4		vis	0.00089308		vis=exp(-10.547 + 541.69 / (T - 144.53))	Liquid viscosity (Pa-s)
5		Re	88620.3631		Re=D * v * rho / vis	Reynold's number
6		v	1.98943214		v=q / (pi * D ^ 2 / 4)	Flow velocity (m/s)
7		dp	103000		dp=103000	Pressure drop (Pa)
8		L	100		L=100	Pipe length (m)
9		T	298.15		T=25 + 273.15	Temperature (K)
10		pi	3.1416		pi=3.1416	
11		q	0.0025		q=0.0025	Flow rate (cu-m/s)
12	Implicit Vars	D	0.04		D(0)=0.04	Calculation of pipe diameter for specified flowrate
13		fF	0.004		fF(0)=0.004	Fanning's friction factor
14	Implicit Eqs	f(D)	24272.8979		f(D)=dp - 2 * fF * rho * v * v * L / D	
15		f(fF)	-0.000695		f(fF)=If (Re < 2100) Then (fF - 16 / Re) Else (fF - 1 / (4 * log(Re * sqrt(fF)) - 0.4) ^ 2)	
16	Sum of Squares:		589173571		F = f(D)^2+f(fF)^2	

The same Excel spreadsheet from above with the visible cell contents is shown below.

	A	B	C	D	
1	POLYMATH				
2		Variable	Value		Polymath Eq
3	Explicit Eqs	rho	=(46.048 + (C9 * (9.418 + (C9 * (-0.0329 + (C9 * (0.00004882 - (C9 * 0.00000002895))))))))		rho=46.048 +
4		vis	=EXP((-10.547 + (541.69 / (C9 - 144.53))))		vis=exp(-10.5
5		Re	=(((C12 * C6) * C3) / C4)		Re=D * v * rho
6		v	=(C11 / ((C10 * (C12 ^ 2)) / 4))		v=q / (pi * D ^
7		dp	=103000		dp=103000
8		L	=100		L=100
9		T	=(25 + 273.15)		T=25 + 273.15
10		pi	=3.1416		pi=3.1416
11		q	=0.0025		q=0.0025
12	Implicit Vars	D	0.04		D(0)=0.04
13		fF	0.004		fF(0)=0.004
14	Implicit Eqs	f(D)	=(C7 - ((((((2 * C13) * C3) * C6) * C6) * C8) / C12))		f(D)=dp - 2 * fi
15		f(fF)	=IF((C5 < 2100),(C13 - (16 / C5)),(C13 - (1 / (((4 * LOG10((C5 * SQRT(C13)))) - 0.4) ^ 2))))		f(fF)=If (Re < 2
16	Sum of Squares:		=((C14 ^ 2) + (C15 ^ 2))		F = f(D)^2+f(fF

For systems of nonlinear equations, the Excel Add-In named Solver (Provided within Excel) is used to minimize the "Sum of Squares" as is shown below



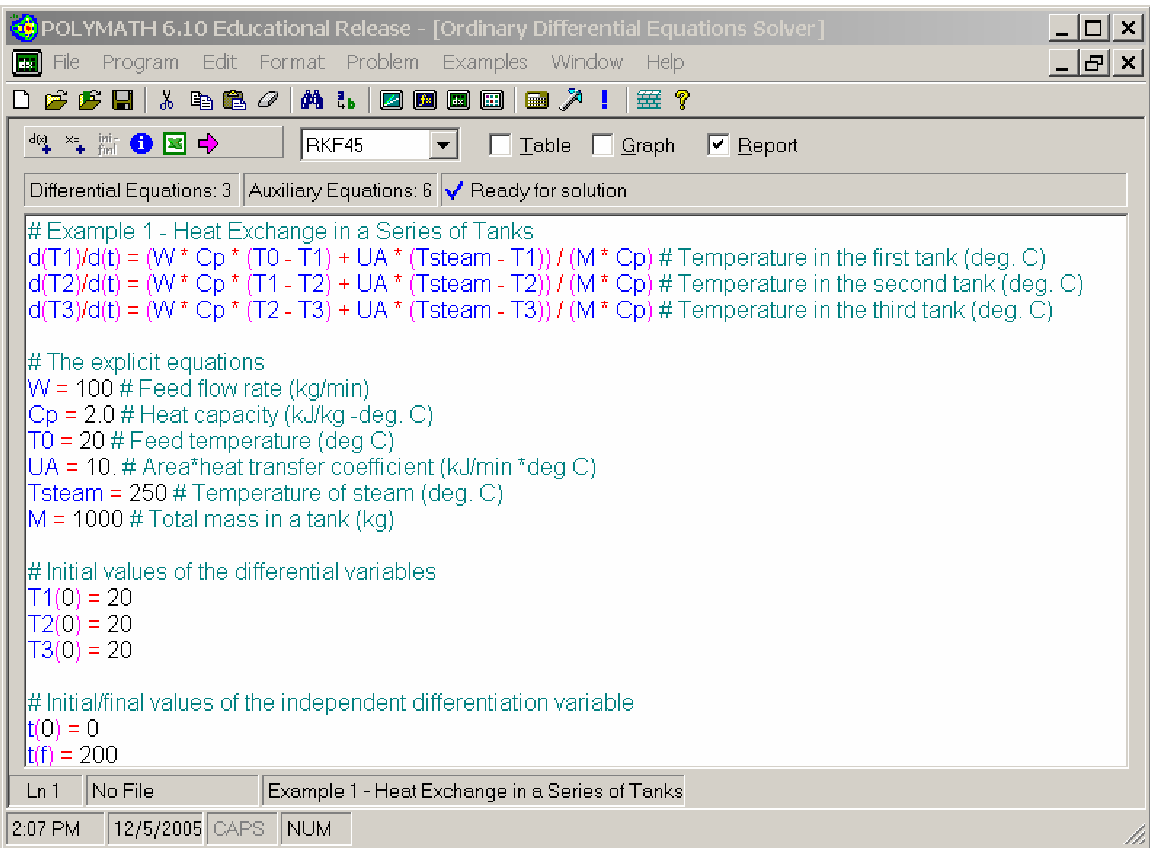
where the solution is

12	Implicit Vars	D	0.03952106	D(0)=0.04	Calculation of pipe diameter for specified flowrate
13		fF	0.00492738	fF(0)=0.004	Fanning's friction factor
14	Implicit Eqs	f(D)	0.00374439	f(D)=dp - 2 * fF * rho * v * v * L / D	
15		f(fF)	0.00035971	f(fF)=If (Re < 2100) Then (fF - 16 / Re) Else (fF - 1 / (4 * log(Re * sqrt(fF)) - 0.4) ^ 2)	
16	**Sum of Squares:**		1.415E-05	F = f(D)^2+f(fF)^2	
17					

POLYMATH Example 1 for the Ordinary Differential Equations Solver

EXCEL does not have the capabilities to solve systems of ordinary differential equations, so POLYMATH provides an ODE_Solver program for Excel that provides this capability. Once installed in Excel, this Add-In can be used to easily solve problems involving ordinary differential equations within Excel. The same choice of integration algorithms and control of the integration is provided, and the results compare directly with those of POLYMATH as the same solution coding is used.

Consider Example 1 from the POLYMATH Differential Equation Solver.

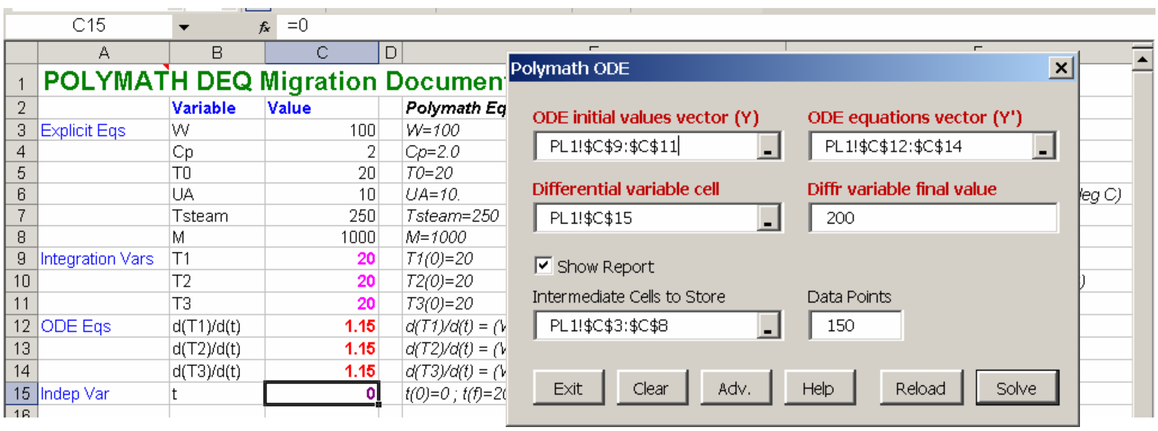


A single key press on the Excel icon automatically exports this problem to Excel.

C15 =0

	A	B	C	D	E	F
1	**POLYMATH DEQ Migration Document**					
2		**Variable**	**Value**		***Polymath Equation***	***Comments***
3	Explicit Eqs	W	100		*W=100*	*Feed flow rate (kg/min)*
4		Cp	2		*Cp=2.0*	*Heat capacity (kJ/kg -deg. C)*
5		T0	20		*T0=20*	*Feed temperature (deg C)*
6		UA	10		*UA=10.*	*Area*heat transfer coefficient (kJ/min *deg C)*
7		Tsteam	250		*Tsteam=250*	*Temperature of steam (deg. C)*
8		M	1000		*M=1000*	*Total mass in a tank (kg)*
9	Integration Vars	T1	**20**		*T1(0)=20*	*Temperature in the first tank (deg. C)*
10		T2	**20**		*T2(0)=20*	*Temperature in the second tank (deg. C)*
11		T3	**20**		*T3(0)=20*	*Temperature in the third tank (deg. C)*
12	ODE Eqs	d(T1)/d(t)	**1.15**		*d(T1)/d(t) = (W * Cp * (T0 - T1) + UA * (Tsteam - T1)) / (M * Cp)*	
13		d(T2)/d(t)	**1.15**		*d(T2)/d(t) = (W * Cp * (T1 - T2) + UA * (Tsteam - T2)) / (M * Cp)*	
14		d(T3)/d(t)	**1.15**		*d(T3)/d(t) = (W * Cp * (T2 - T3) + UA * (Tsteam - T3)) / (M * Cp)*	
15	Indep Var	t	0		*t(0)=0 ; t(f)=200*	

The POLYMATH ODE_Solver Add-In within Excel presents a control display as shown. Note that no other Excel Add-In is available for Excel that permits the solution of simultaneous ordinary differential equations. This is a unique capability of POLYMATH 6, and this Add-In software is provided to POLYMATH users. It can also be used entirely separately from POLYMATH.



The solution is automatically presented as a new Excel worksheet which is partially shown below

L20

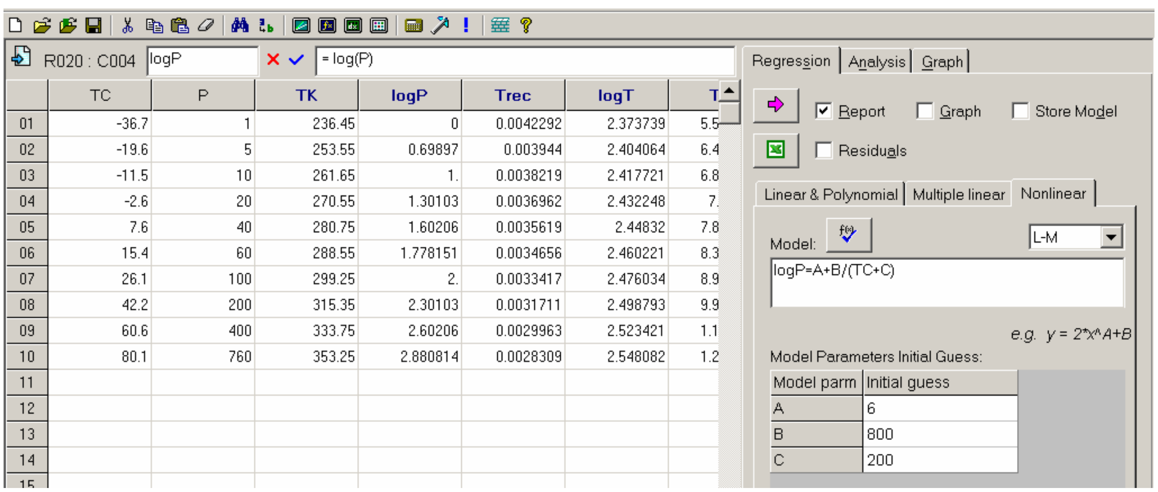
	A	B	C	D	E	F
1	**POLYMATH Report DEQ**					
2	Ordinary Differential Equations (RKF45).					
3						
4	**Calculated values of DEQ variables**					
5		Variable	Initial	Minimal	Maximal	Final
6	1	t	0	0	200	200
7	2	T1	20	20	30.95238	30.95238
8	3	T2	20	20	41.38322	41.38322
9	4	T3	20	20	51.31735	51.31735
10	5	W	100	100	100	100
11	6	Cp	2	2	2	2
12	7	T0	20	20	20	20
13	8	UA	10	10	10	10
14	9	Tsteam	250	250	250	250
15	10	M	1000	1000	1000	1000

35	**Intermediate data points**										
36		t	T1	T2	T3	W	Cp	T0	UA	Tsteam	M
37	1	0	20	20	20	100	2	20	10	250	1000
38	2	3.319887	23.22346	23.72752	23.78164	100	2	20	10	250	1000
39	3	4.386554	24.04239	24.86117	24.97617	100	2	20	10	250	1000
40	4	5.453221	24.77454	25.95281	26.1564	100	2	20	10	250	1000
41	5	7.586554	26.01434	27.99601	28.46225	100	2	20	10	250	1000
42	6	8.653221	26.53755	28.94355	29.5821	100	2	20	10	250	1000
43	7	9.719887	27.00533	29.84058	30.67631	100	2	20	10	250	1000
44	8	10.78655	27.42354	30.68718	31.74251	100	2	20	10	250	1000
45	9	12.91989	28.13173	32.23198	33.78281	100	2	20	10	250	1000
46	10	13.98655	28.43059	32.93261	34.75364	100	2	20	10	250	1000
47	11	15.05322	28.69779	33.58751	35.68995	100	2	20	10	250	1000
48	12	16.11989	28.93668	34.1985	36.59086	100	2	20	10	250	1000
49	13	18.25322	29.3412	35.29665	38.28444	100	2	20	10	250	1000

These tables give an overview of the solution and then the numerical results for printing or plotting with Excel. Additional problem solving is possible from within Excel.

POLYMATH Example 2 for the Regression Program (Nonlinear Regression)

For the general nonlinear regression which is only one of the many regression options, the POLYMATH program entry is shown as follows for the fitting of the Antoine Equation to vapor pressure data. The Model equation as shown below is provided by the user and can utilize any of the columns of the Data Table.

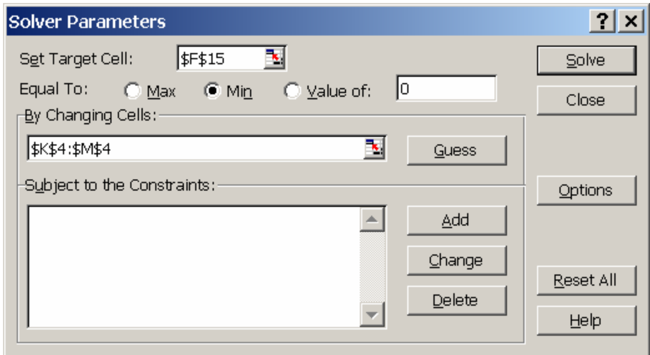


	TC	P	TK	logP	Trec	logT	T
01	-36.7	1	236.45	0	0.0042292	2.373739	5.5
02	-19.6	5	253.55	0.69897	0.003944	2.404064	6.4
03	-11.5	10	261.65	1.	0.0038219	2.417721	6.8
04	-2.6	20	270.55	1.30103	0.0036962	2.432248	7.
05	7.6	40	280.75	1.60206	0.0035619	2.44832	7.8
06	15.4	60	288.55	1.778151	0.0034656	2.460221	8.3
07	26.1	100	299.25	2.	0.0033417	2.476034	8.9
08	42.2	200	315.35	2.30103	0.0031711	2.498793	9.9
09	60.6	400	333.75	2.60206	0.0029963	2.523421	1.1
10	80.1	760	353.25	2.880814	0.0028309	2.548082	1.2

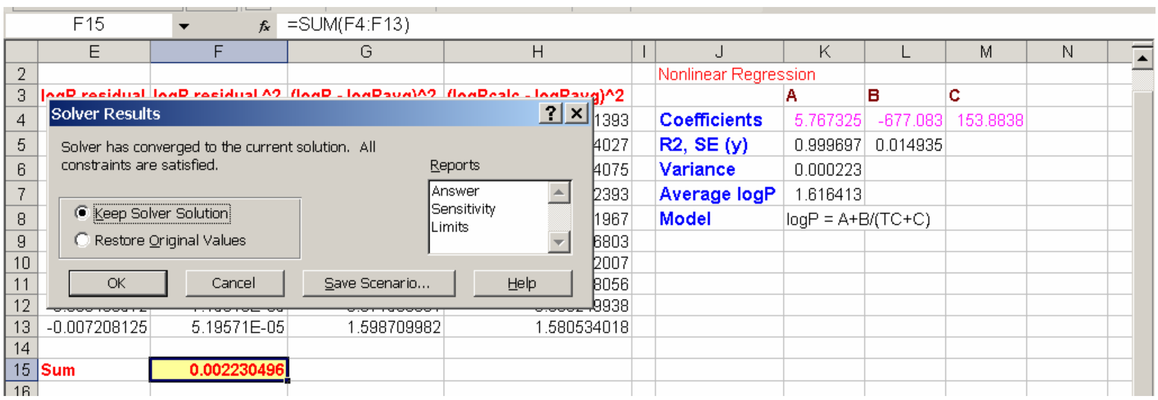
A mouse click on the Excel icon results in the automatic export to Excel as shown.

	E	F	G	H	I	J	K	L	M	N
1	**linear Regression Migration Document**									
2						Nonlinear Regression				
3	**logP residual**	**logP residual ^2**	**(logP - logPavg)^2**	**(logPcalc - logPavg)^2**			**A**	**B**	**C**	
4	1.101041029	1.212291347	4.855357224	1.215388253		**Coefficients**	6	-800	200	
5	0.8664402	0.750718619	2.26357295	0.407142659		**R2, SE (y)**	0.341839	0.636649		
6	0.75596817	0.571487874	1.448382196	0.200273563		**Variance**	0.405322			
7	0.646285096	0.417684426	0.814429564	0.065624308		**Average logP**	2.203488			
8	0.544375453	0.296344634	0.361715054	0.003254938		**Model**	logP = A+B/(TC+C)			
9	0.507828573	0.257889859	0.18091115	0.00680494						
10	0.461742592	0.213206221	0.041407168	0.066695685						
11	0.395914674	0.156748429	0.009514537	0.243499969						
12	0.328101167	0.107650375	0.158860027	0.528054597						
13	0.263063187	0.06920224	0.458771169	0.884332737						
14										
15	**Sum**	**4.053224025**								

The Excel Add-In Solver is used to minimize the Sum of Squares objective function which has been automatically created by POLYMATH.



The Solver results are shown below.



Similar capabilities are available for Linear Regression, Polynomial Curve Fitting, and Multiple Linear Regression.

SUMMARY

The latest POLYMATH 6 software package that is available to academic departments via inexpensive site licenses through CACHE provides unique capabilities that promote the use of Excel and MATLAB.

The problem exports from POLYMATH to Excel described in this article allow for very efficient problem solving within Excel that also allows solution verification with the POLYMATH solutions. This capability may be very useful in teaching problem solving to undergraduate. The initial use of POLYMATH can lead to the development of problem solving skills with Excel. This is particularly important as recent CACHE survey has indicated that Excel is the calculational tool of choice for practicing chemical engineers.

A very unique capability for Excel is provided by the POLYMATH ODE_Solver Add-In which enables the effective solution of problems involving ODE's completely within Excel. No other Add-In software enables this convenient capability.

The Spring CACHE Newsletter will highlight the POLYMATH capability to generate MATLAB "M" files automatically from POLYMATH programs.

Recent papers on POLYMATH are available from the website:

http://www.polymath-software.com/

Questions above POLYMATH may be directed to the academic authors.

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