Polymath Software Report

Michael B. Cutlip CACHE Trustee's Meeting Notre Dame University June 19, 2014

POLYMATH – Brief History

- CACHE Site Licenses Started in 1990
- Polymath Software 2014
 Currently ~ 125+ paid CACHE site licenses plus ~ 40 institutions in developing countries, used with seven textbooks, personal educational and professional versions available via Internet sales
- Himmelblau Award of CAST Division to authors 2010

Current CACHE Site Licenses (now into 25th year)

Site licenses for POLYMATH software are available through the CACHE Corporation to academic departments (mostly CHEG) to some engineering colleges and schools. Computer labs, networks, faculty, and staff receive copies on an annual basis.

Current CACHE supporting departments pay \$175 for the first year and \$125 for each successive year thereafter. CACHE nonmember institution rates are an initial \$300 for the first year and a \$250 annual fee for subsequent years.

POLYMATH Individual Educational Licenses

- Internet Sales Currently4-months \$2012-months \$30Unlimited use \$39
- Special Sales with Textbooks Using Polymath at 50% of the Prices Given Above Thus a student with the latest Cutlip, Fogler, and Himmelblau books can get over a semester of unlimited use for ONLY \$10.

POLYMATH Individual Professional License

■ Unlimited use \$189

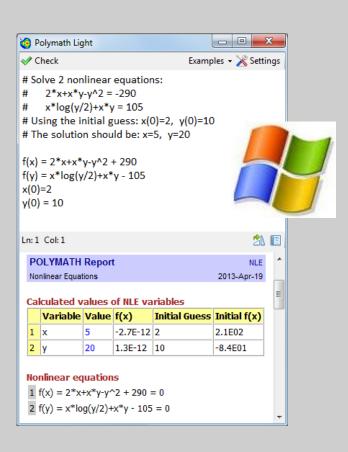
POLYMATH Current Activities

- POLYMATH 6.2 Educational Site License Version now included Limited DIPPR Database and User Interface at no cost.
- DIPPR Add-On May be made Available
 - Educational Site License Add-On \$700/YR
 - Single User Educational License Add-On \$100/YR
 - Single User Professional License Add-On \$300/YR
- POLYMATH 7 under Development and Class Testing Underway Completely .NET 4.0 code

POLYMATH 7 Coming in 2014

- 1. Linear Programming New Simplex Solver
- 2. Nonlinear Equations Automated Creation of complete MATLAB m-files
- 3. Differential Equations Output Options, Creation of MATLAB m-file, Tabular Outputs at Desired Intervals, Export to Excel with ODE Solver Add-In
- 4. Simulation with Parameter Estimation in Dynamical Systems
- 5. DIPPR Database Interface for Constant and Variable Properties with output to Polymath, MATLAB and Excel

PolyMathLite is Coming to Android is here!!!!! www.polymathlite.com





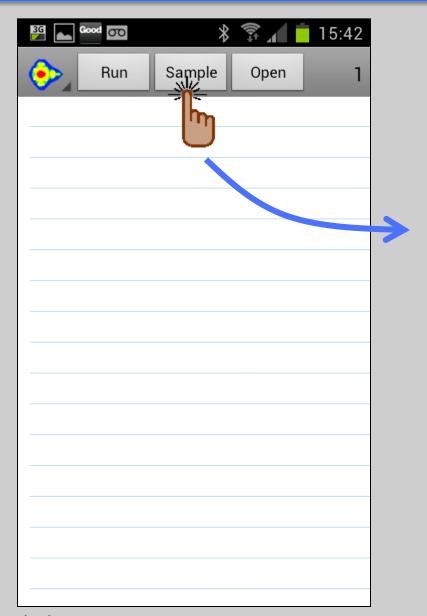
Android Based PolyMathLite

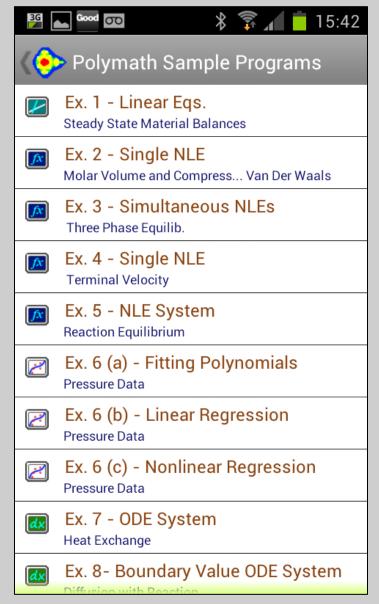


Same program syntax for NLE, DEQ Simplified Syntax for LEQ Simplified Syntax for REG Access to Chart Software Direct Conversion to Matlab Sharing Options via E-mail and Bluetooth

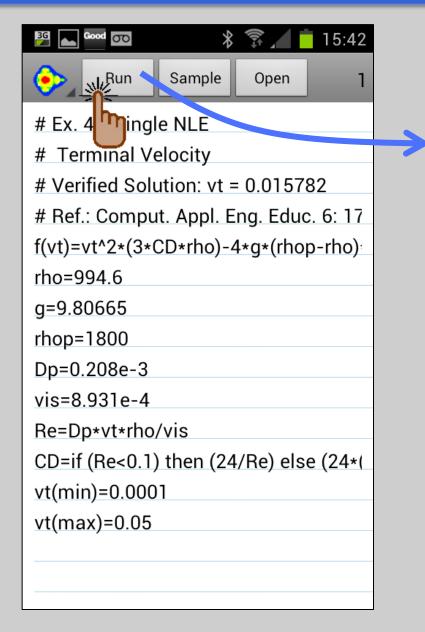


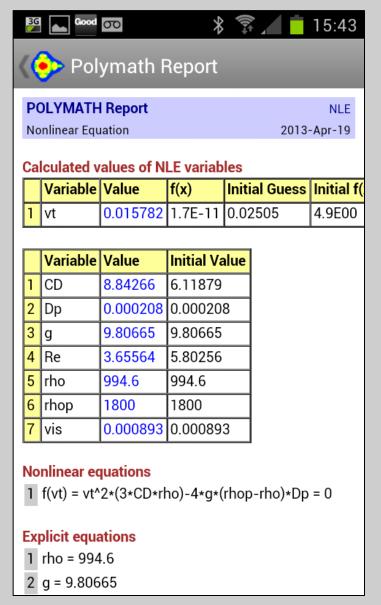
Home Screen, Open Sample





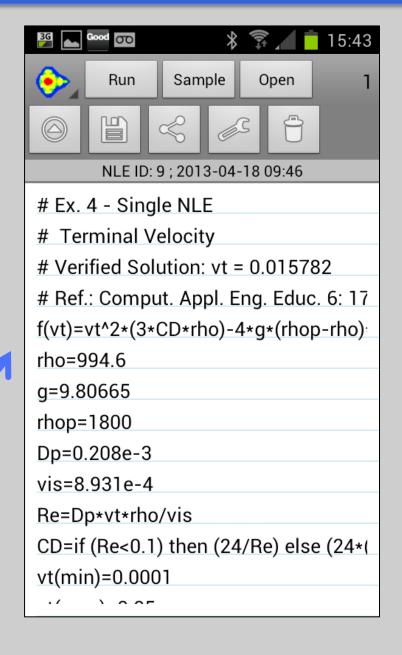
Edit Program, Run Program, Get Solution Report





Open Saved File, Save/Share/Settings Buttons

3G 🛌 G	ood 50	3 🕏 📶 📋 15:43
Open Pol	ymath File	
Ex. 1 - Li	inear Eqs.	
LEQ	2	2013-04-18 00:38
Ex. 2 - S	ingle NLE	
NLE	6	2013-04-18 09:46
Ex. 2 - S	ingle NLE	
NLE	7	2013-04-18 09:46
Ex. 3 - S	imultaneous NLEs	
NLE	1	2013-04-18 00:38
Ex. 3 - S	imultaneous NLEs	
NLE	8	2013-04-18 09:46
Ex. 4 - S	ingle NLE	
NLE	9	2013-04-18 09:46
Ex. 4 - S	ingle NLE	
NLE	10	2013-04-18 09:46
Ex. 5 - N	LE System	
NLE	3	2013-04-18 00:38
Ex. 5 - N	LE System	
NLE	5	2013-04-18 01:12
F _Y 6 (b)	Linear Degraceia	



Settings Screen









Polymath Light for Android

Polymath is a proven computational system, which has been specifically created for educational or professional use. It allows the user to apply effective numerical analysis techniques during interactive problem solving on Android OS smart phones and Tablets.

Results are presented with a standard html based report for easy understanding and can be shared across for incorporation into mail messages, papers, and reports. Students, engineers, mathematicians, scientists, or anyone with a need to problems will appreciate the efficiency and speed of problem solution.

This Help will enable you to start using Polymath for engineering problem solving. For advanced applications please refer also to PolyMathLite User's Manual which is available at the website: www.polymathlite.com

Content:







applications picase relei also to i olymatricite osers imarida website:www.polymathlite.com

Content:



Main Problem Entry Screen **Linear Equations Nonlinear Equations** Ordinary Differential Equations Polynomial Regression Multiple linear Regression Nonlinear Regression Polymath Control Buttons Built in Samples Screen Variables and Expressions

Main Problem Entry Screen





Polymath Help

	exp(o = o + 10g(o))
Condition Operator	These operators return "1" if the condition met, and "0" if the condition does not meet. Examples: The expression '3>6' returns 0. The expression '4>=4' returns 1. Valid conditional operators:
	>, <, >=, <=, ==
Boolean	The Boolean operators return "1" if the condition is met, and "0" if the condition is not met. Example: The expression '(2>3) or (1>0)' returns 1. The expression '1 and 0' returns 0.
Operator	Valid Boolean operators: And, Or
If There The	There are three case-insensitive keywords which compose the if-then-else expression structure. The three keywords are: If, Then, Else.
If-Then-Else	Samples: If (2>5) Then (sin(12)+4) Else (sin(12)+8) if(2>5)then(sin(12)+4)else(sin(12)+8)
	Open Parenthesis: (

🐤 Polymath Help

A special 'if' statement is available, with the following syntax:

```
if (condition) then (expression1) else (expression2)
```

The parentheses are optional.

The condition may include the following operators: and, or (Boolean operators), > (greater than), < (less than), >= (greater than or equal), <= (less than or equal), == (equals).

The expressions may be any formula, including another 'if' statement.

For example:

```
A = if (x>0) then (log(x)) else(0)
b = if (T<minT) then (minT) else (if (T>maxT) then (maxT) else
(T))
Vol h1 = if (a>5 and c<2) then 1.12 else 7.89
```

Available Functions







Available Functions

A number of standard functions are available for use in the various programs. The arguments of the functions must be enclosed in parentheses. The arguments may be themselves expressions or other functions. The nesting of functions is allowed.

Function Name	Description	
abs()	absolute value	
arccos()	trigonometric inverse cosine with result in radians	
arccosec ()	trigonometric inverse cosecant with result in radians	
arccosech ()	inverse hyperbolic cosecant	
arcsech ()	inverse hyperbolic secant	
arccosh ()	inverse hyperbolic cosine	
arccotan ()	trigonometric inverse cotangent with result in radians	
arccotanh ()	inverse hyperbolic cotangent	
orocco ()	trigonometric inverse eccent with regult in rediene	







	,
cosec()	trigonometric cosecant with argument in radians
cosech()	hyperbolic cosecant
cosh()	hyperbolic cosine
cotan ()	trigonometric cotangent with argument in radians
coth()	hyperbolic cotangent
exp()	exponential (e^x)
erf () error function	
exp10 () exponential of 10 (10 ^x)	
exp2 () exponential of 2 (2^x)	
fact (N) factorial of integer part of number N (this only operates on a nu	
frac ()	fractional part
int ()	integer part
In () natural logarithm to the base e	
log () logarithm to the base 10	
psi () psi function	



(Polymath Sample Programs



Ex. 2 - Single NLE

Molar Volume and Compress... Van Der Waals

Ex. 3 - NLE System
Three Phase Equilib.

Ex. 4 - Single NLE
Terminal Velocity

Ex. 5 - NLE System
Reaction Equilibrium

Ex. 6 (a) - Fitting Polynomials
Pressure Data

Ex. 6 (b) - Linear Regression
Pressure Data

Ex. 6 (c) - Nonlinear Regression
Pressure Data

Ex. 7 - ODE System
Heat Exchange

Ex. 8- Boundary Value ODE System
Diffusion with Reaction

Ex. 9 - ODE System

Reversible Reaction in a PBR



NLE





POLYMATH Report

Nonlinear Equation 2013-Jun-14

Calculated values of NLE variables

	Variable	Value	f(x)	Initial Guess	Initial f(x)
1	٧	0.574892	9.5E-11	0.7	5.9E00

	Variable	Value	Initial Value	
1	а	4.19695	4.19695	
2 b 0.037		0.037371	0.037371	
3	Р	56	56	
4	Pc	111.3	111.3	
5	Pr	0.503145	0.503145	
۾	Ь	ก กฎวกผ	U U83UE	







	Variable	Value	f(x)	Initial Guess	Initial f(x)
1	٧	0.574892	9.5E-11	0.7	5.9E00

	Variable	Value	Initial Value
1	а	4.19695	4.19695
2	b	0.037371	0.037371
3 P		56	56
4 Pc 111.3 1		111.3	
5	Pr	0.503145	0.503145
6	R	0.08206	0.08206
7	Т	450	450
8	Тс	405.5	405.5
9	9 Z 0.871		1.06155



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Nonlinear equations

1
$$f(V) = (P+a/(V^2))*(V-b)-R*T = 0$$

Explicit equations

- 1 P = 56
- 2 R = 0.08206
- 3 T = 450
- 4 Tc = 405.5
- 5 Pc = 111.3
- 6 Pr = P/Pc
- $7 a = 27*(R^2*Tc^2/Pc)/64$
- 8 b = R*Tc/(8*Pc)
- 9 Z = P*V/(R*T)







Problem source text

```
# Ex. 2 - Single NLE
# Molar Volume and Compress... Van Der Waals
# Verified Solution: V=0.574892, Z =0.871827
# Ref.: Comput. Appl. Eng. Educ. 6: 171-172, 1998
f(V)=(P+a/(V^2))*(V-b)-R*T
P=56
R=0.08206
T=450
Tc=405.5
Pc=111.3
Pr=P/Pc
a=27*(R^2*Tc^2/Pc)/64
b=R*Tc/(8*Pc)
Z=P*V/(R*T)
```





Matlab formatted problem

Create m file called PolyNle.m and paste the following text into it.

```
% Polymath NLE problem conversion to Matlab
% NLE
function PolyNle
 xguess = 0.7;
 x = fzero(@NLEfun,xguess);
 fprintf('The NLE solution is %g\n', x);
end
function fV = NLEfun(V)
 P = 56:
 R = 0.08206;
 T = 450;
 Tc = 405.5;
 Pc = 111.3;
 Pr = P / Pc:
 a = 27 * R ^ 2 * Tc ^ 2 / Pc / 64;
 b = R * Tc / (8 * Pc);
 Z = P * V / (R * T);
 fV = (P + a / (V ^ 2)) * (V - b) - (R * T);
end
```







🐤 Polymath Report

```
Pr = P / Pc;

a = 27 * R ^ 2 * Tc ^ 2 / Pc / 64;

b = R * Tc / (8 * Pc);

Z = P * V / (R * T);

fV = (P + a / (V ^ 2)) * (V - b) - (R * T);

end
```

General Settings

Total number of equations 10 Number of implicit equations 1 Number of explicit equations 9

Elapsed time 0.07 sec

Reporting digits 8

Solution method safenewt

Max iterations 150
Tolerance F 1E-07
Tolerance X 1E-07
Tolerance min 1E-07

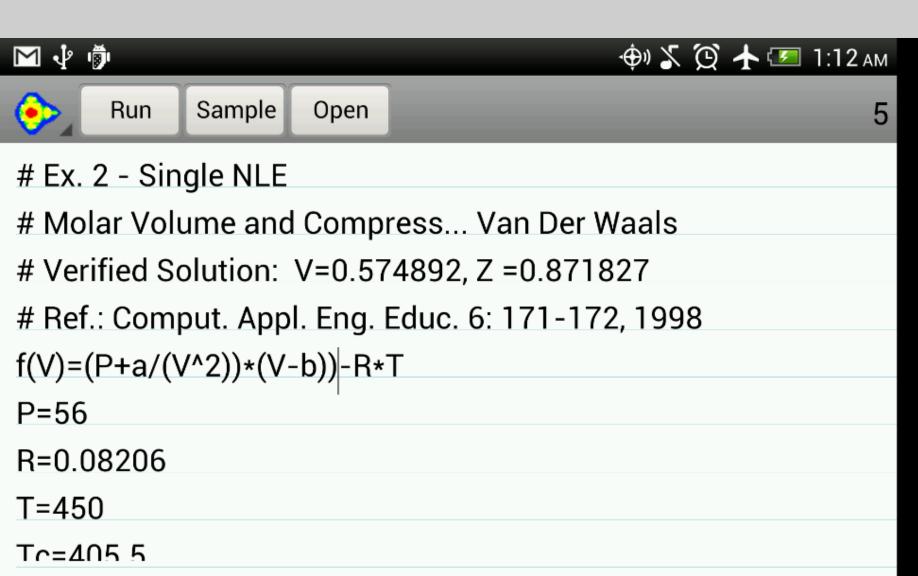
Data file: no file



```
🚓) 🗴 💢 🛧 🕶 1:12 ам
```

```
# Ex. 2 - Single NLE
# Molar Volume and Compress... Van Der
Waals
# Verified Solution: V=0.574892, Z =0.871827
# Ref.: Comput. Appl. Eng. Educ. 6: 171-172,
1998
f(V)=(P+a/(V^2))*(V-b))-R*T
P = 56
R=0.08206
T = 450
Tc = 405.5
Da-111 2
```

Done









Errors in NLE

	Message
1	Error in Line #5, unequal number of parantheses. Too many ')'
2	Implicit variables (1) V
3	Explicit variables (9) P, R, T, Tc, Pc, Pr, a, b, Z
4	All variables (10) P, a, V, b, R, T, Tc, Pc, Pr, Z



```
🚓) 🗴 💢 🛧 🛂 1:14 ам
```

```
# Ex. 2 - Single NLE
# Molar Volume and Compress... Van Der
Waals
# Verified Solution: V=0.574892, Z =0.871827
# Ref.: Comput. Appl. Eng. Educ. 6: 171-172,
1998
f(V)=(P+a/(V^2))*(v-b)-R*T
P = 56
R=0.08206
T = 450
Tc = 405.5
Da-111 2
```

Done







Errors in NLE

	Message
1	1 Undefined variable exists; v
2	Implicit variables (1) V
3	Explicit variables (9) P, R, T, Tc, Pc, Pr, a, b, Z
4	All variables (11) P, a, V, v, b, R, T, Tc, Pc, Pr, Z







🤥 Polymath Sample Programs



Ex. 12 - Single Partial Diff. Eq. Unsteady State Heat Conduction.



Ex. 13 - Nonlinear Regression
Catalytic Reforming Reac.



Ex. 14(a) - Multi-Linear Regression
Heat of Hardening



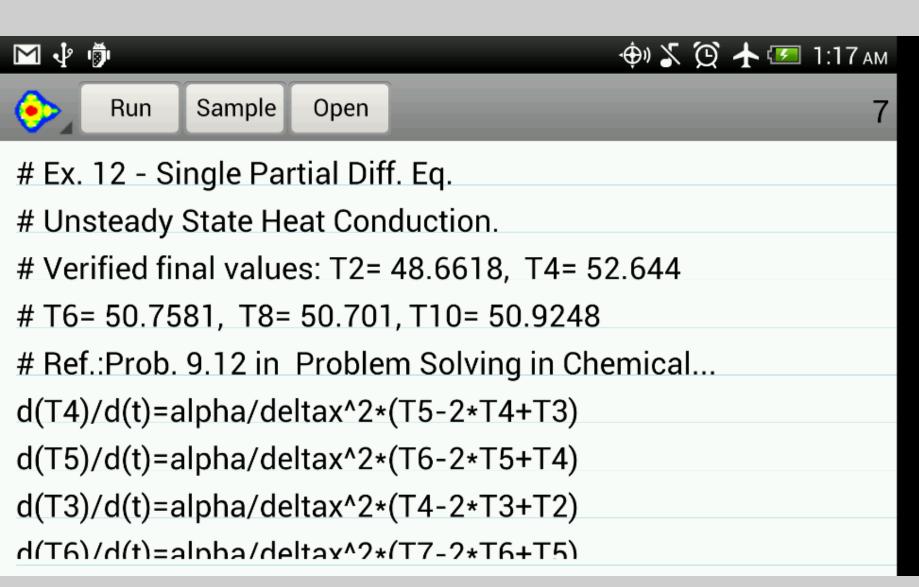
Ex. 14(b) - Multi-Linear Regression via origin
Heat of Hardening

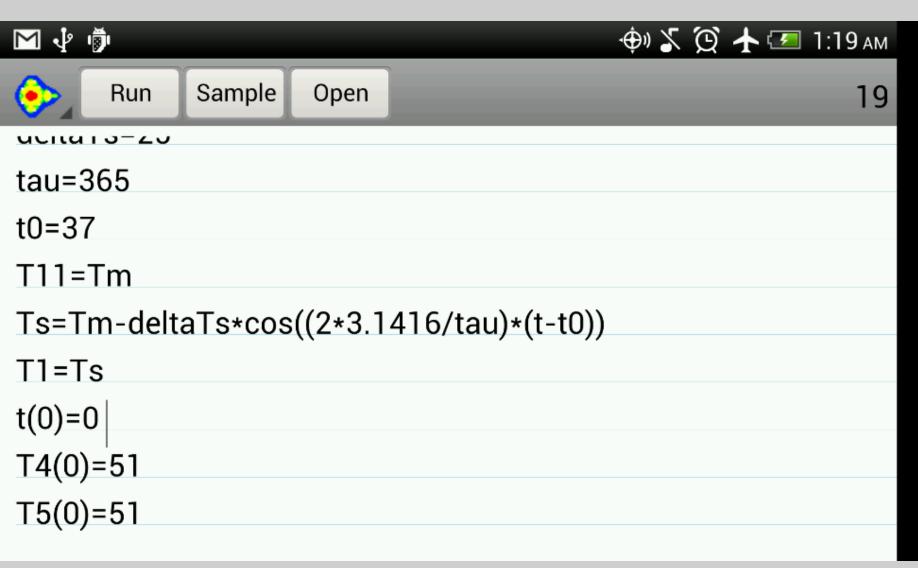


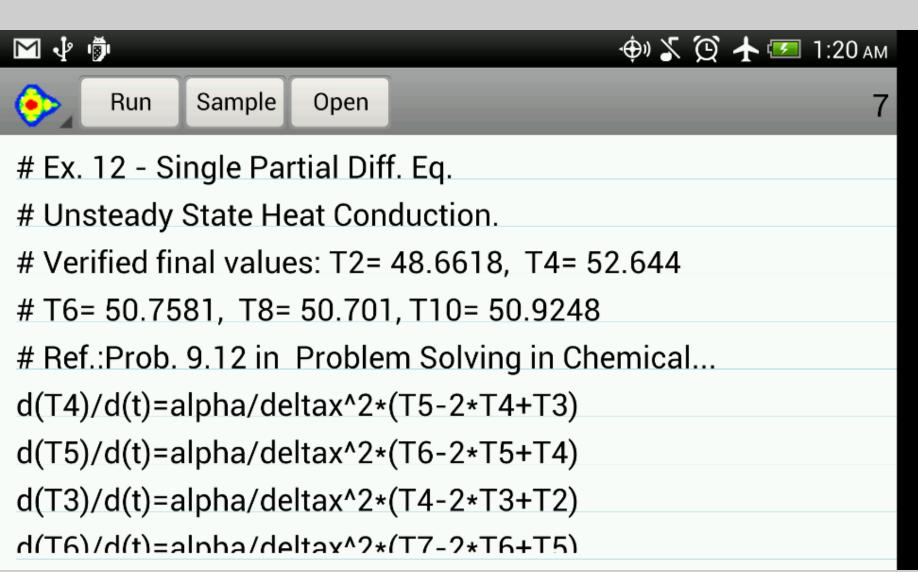
Ex. 15 - Linear Eqs. Biological Reactors



Ex. 16 - Stiff ODE System Biological Reactors











POLYMATH Report

Ordinary Differential Equations

DEQ

2013-Jun-14

Calculated values of DEQ variables

	Variable	Initial value	Final value	Minimal value	Maximal value
1	alpha	0.9	0.9	0.9	0.9
2	deltaTs	25	25	25	25
3	deltax	8	8	8	8
4	t	0	365	0	365
5	t0	37	37	37	37
6	T1	30.9018	30.9016	26.0001	75.9937
7	T10	51	50.9248	50.9248	51
8	T11	51	51	51	51
a	T2	51	48 6618	30 6826	61 7570



🐤 Polymath Report

Differential equations

- $d(T4)/d(t) = alpha/deltax^2*(T5-2*T4+T3)$
- $d(T5)/d(t) = alpha/deltax^2*(T6-2*T5+T4)$
- $3 d(T3)/d(t) = alpha/deltax^2*(T4-2*T3+T2)$
- $d(T6)/d(t) = alpha/deltax^2*(T7-2*T6+T5)$
- $d(T2)/d(t) = alpha/deltax^2*(T3-2*T2+T1)$
- $d(T7)/d(t) = alpha/deltax^2*(T8-2*T7+T6)$
- $d(T8)/d(t) = alpha/deltax^2*(T9-2*T8+T7)$
- $d(T9)/d(t) = alpha/deltax^2*(T10-2*T9+T8)$
- $d(T10)/d(t) = alpha/deltax^2*(T11-2*T10+T9)$

Explicit equations

- alpha = 0.9



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Problem source text

```
# Ex. 12 - Single Partial Diff. Eq.
# Unsteady State Heat Conduction.
# Verified final values: T2= 48.6618, T4= 52.644
# T6= 50.7581, T8= 50.701, T10= 50.9248
# Ref.:Prob. 9.12 in Problem Solving in Chemical..
d(T4)/d(t)=alpha/deltax^2*(T5-2*T4+T3)
d(T5)/d(t)=alpha/deltax^2*(T6-2*T5+T4)
d(T3)/d(t)=alpha/deltax^2*(T4-2*T3+T2)
d(T6)/d(t)=alpha/deltax^2*(T7-2*T6+T5)
d(T2)/d(t)=alpha/deltax^2*(T3-2*T2+T1)
d(T7)/d(t)=alpha/deltax^2*(T8-2*T7+T6)
d(T8)/d(t)=alpha/deltax^2*(T9-2*T8+T7)
d(T9)/d(t)=alpha/deltax^2*(T10-2*T9+T8)
d(T10)/d(t)=alpha/deltax^2*(T11-2*T10+T9)
alpha=0.9
deltax=8
Tm=51
```





Matlab formatted problem

Create m file called PolyOde.m and paste the following text into it.

```
% Polymath ODE problem conversion to Matlab
% DEQ
function PolyOde
  tspan = [0 365]; % Range for the independent variable
  y0 = [51; 51; 51; 51; 51; 51; 51; 51; 51]; % Initial values for the dependent variables
  [t,y]=ode45(@ODEfun,tspan, y0);
  plot (t,y);
  xlabel('t');
  legend('T4','T5','T3','T6','T2','T7','T8','T9','T10');
  fprintf('T4 = %16.6f \n',y(length(y),1));
  fprintf(T5 = \%16.6f \n',y(length(y),2));
  fprintf('T3 = %16.6f \n',y(length(y),3));
  fprintf('T6 = %16.6f \n',y(length(y),4));
  fprintf('T2 = %16.6f \n',y(length(y),5));
  fprintf('T7 = %16.6f \n',y(length(y),6));
  fprintf('T8 = %16.6f \n',y(length(y),7));
  fprintf('T9 = %16.6f \n',y(length(y),8));
  fprintf('T10 = %16.6f \n',y(length(y),9));
end
function dYfuncvecdt = ODEfun(t,Yfuncvec)
```

Polymath Report

```
TI = TIUIICVEC(O),
 T8 = Yfuncvec(7);
 T9 = Yfuncvec(8);
 T10 = Yfuncvec(9);
 alpha = 0.9;
 deltax = 8;
 Tm = 51;
 deltaTs = 25;
 tau = 365;
 t0 = 37;
 T11 = Tm;
 Ts = Tm - (deltaTs * cos(2 * 3.1416 / tau * (t - t0)));
 T1 = Ts;
 dT4dt = alpha / (deltax ^ 2) * (T5 - (2 * T4) + T3);
 dT5dt = alpha / (deltax ^ 2) * (T6 - (2 * T5) + T4);
 dT3dt = alpha / (deltax ^ 2) * (T4 - (2 * T3) + T2);
 dT6dt = alpha / (deltax ^ 2) * (T7 - (2 * T6) + T5);
 dT2dt = alpha / (deltax ^ 2) * (T3 - (2 * T2) + T1);
 dT7dt = alpha / (deltax ^ 2) * (T8 - (2 * T7) + T6);
 dT8dt = alpha / (deltax ^ 2) * (T9 - (2 * T8) + T7);
 dT9dt = alpha / (deltax ^ 2) * (T10 - (2 * T9) + T8);
 dT10dt = alpha / (deltax ^ 2) * (T11 - (2 * T10) + T9);
 dYfuncvecdt = [dT4dt; dT5dt; dT3dt; dT6dt; dT2dt; dT7dt; dT8dt; dT9dt; dT10dt];
end
```

🤛 Polymath Report

General

Total number of equations 18 Number of differential equations 9 Number of explicit equations 9 Reporting digits 8

Elapsed time 0.30 sec Solution method RKF_45 Step size guess. h 1E-06 1E-06 Truncation error tolerance. eps Calculated Intermediate data points 50

Data file: no file

Calculated data points

	t	T4	T5	Т3	Т6	T2	T7	T8	Т9	T10	T11	Ts	T1
1	0	51	51	51	51	51	51	51	51	51	51	30.9018	30.9018
2	16.7188	50.9674	50.9982	50.5598	50.9999	46.8263	51	51	51	51	51	27.9524	27.9524
3	22.5588	50.9273	50.9945	50.2582	50.9997	45.6043	51	51	51	51	51	27.1082	27.1082
4	34.2388	50.7897	50.9765	49.5305	50.9978	43.5003	50.9998	51	51	51	51	26.1195	26.1195



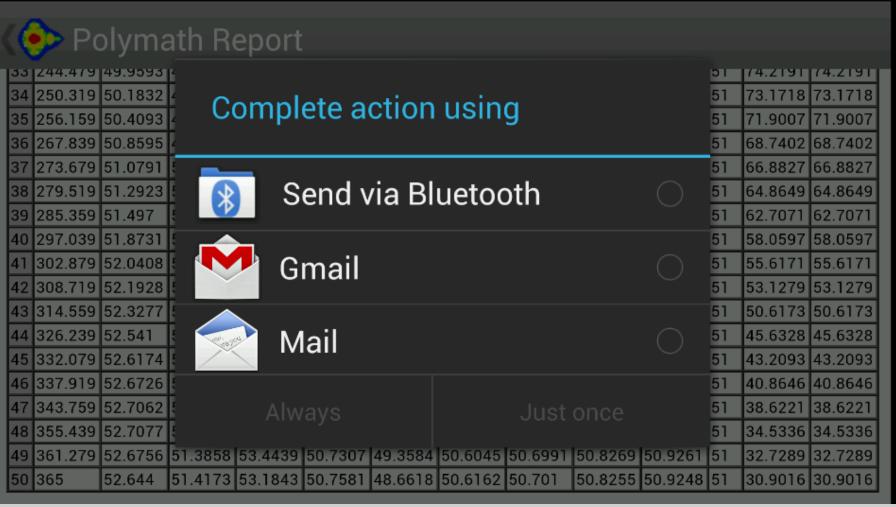


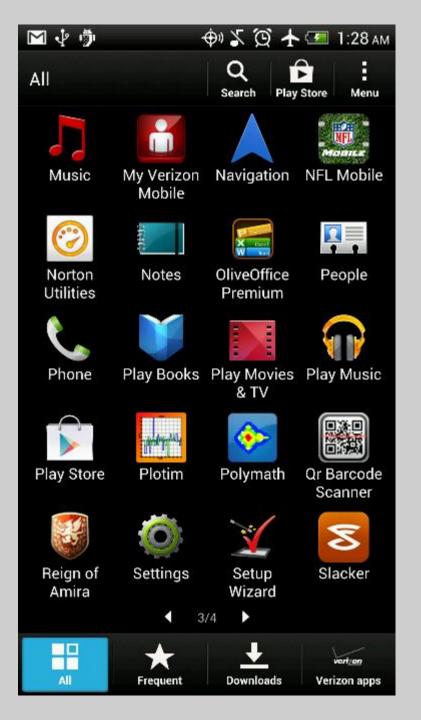


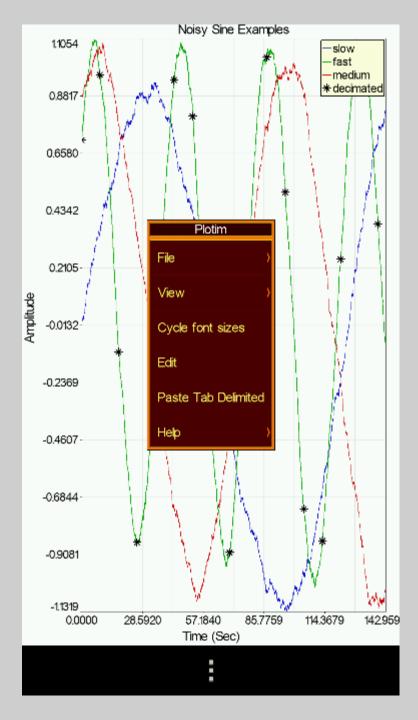
33	244.479	49.9593	49.6506	52.9726	50.1131	01.2082	50.5534	50.8104	50.9297	50.9783	51	74.2191	74.2191
34	250.319	50.1832	49.7177	53.3932	50.1134	61.5561	50.5391	50.7992	50.9238	50.976	51	73.1718	73.1718
35	256.159	50.4093	49.7918	53.7848	50.118	61.7347	50.5262	50.7882	50.9178	50.9737	51	71.9007	71.9007
36	267.839	50.8595	49.9587	54.4654	50.14	61.7579	50.5056	50.7671	50.9056	50.9686	51	68.7402	68.7402
37	273.679	51.0791	50.0499	54.7479	50.1571	61.6025	50.498	50.7573	50.8994	50.966	51	66.8827	66.8827
38	279.519	51.2923	50.1451	54.9879	50.1783	61.3374	50.4922	50.7479	50.8932	50.9633	51	64.8649	64.8649
39	285.359	51.497	50.2435	55.1831	50.2032	60.9655	50.4884	50.7392	50.887	50.9605	51	62.7071	62.7071
40	297.039	51.8731	50.4459	55.4321	50.2634	59.9171	50.4867	50.7236	50.875	50.9549	51	58.0597	58.0597
41	302.879	52.0408	50.5482	55.4835	50.2982	59.2514	50.4888	50.717	50.8692	50.952	51	55.6171	55.6171
42	308.719	52.1928	50.6497	55.4854	50.3357	58.5	50.4929	50.7112	50.8636	50.9492	51	53.1279	53.1279
43	314.559	52.3277	50.7497	55.4379	50.3755	57.6706	50.4988	50.7062	50.8582	50.9463	51	50.6173	50.6173
44	326.239	52.541	50.9411	55.1973	50.4606	55.8119	50.5162	50.6989	50.8483	50.9408	51	45.6328	45.6328
45	332.079	52.6174	51.0307	55.0068	50.5052	54.8016	50.5275	50.6966	50.8438	50.9381	51	43.2093	43.2093
46	337.919	52.6726	51.1151	54.7719	50.5505	53.7507	50.5403	50.6953	50.8396	50.9354	51	40.8646	40.8646
47	343.759	52.7062	51.1935	54.4951	50.5961	52.6699	50.5546	50.6949	50.8358	50.9329	51	38.6221	38.6221
			□ Mai	53.4439					50.8 Co p	y Table	es		
									50.8255	50.9248			

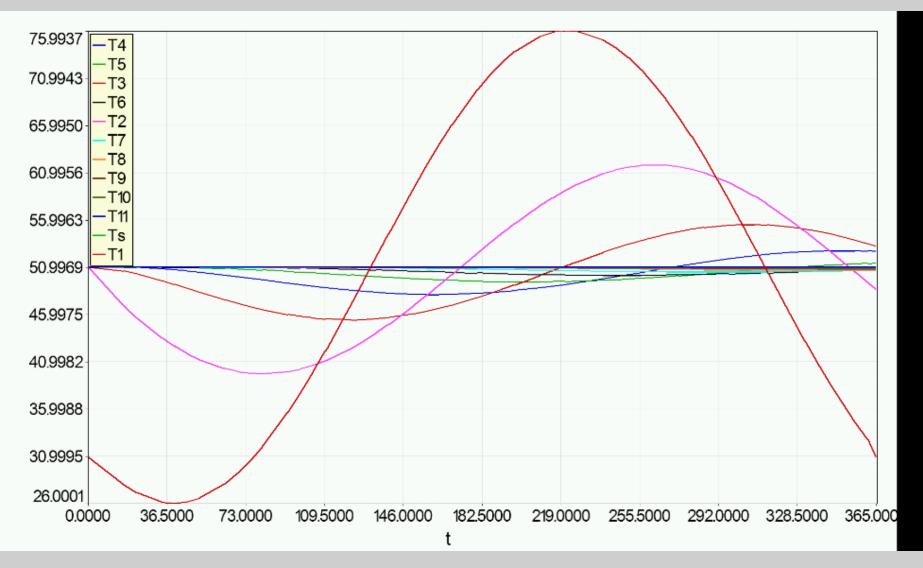


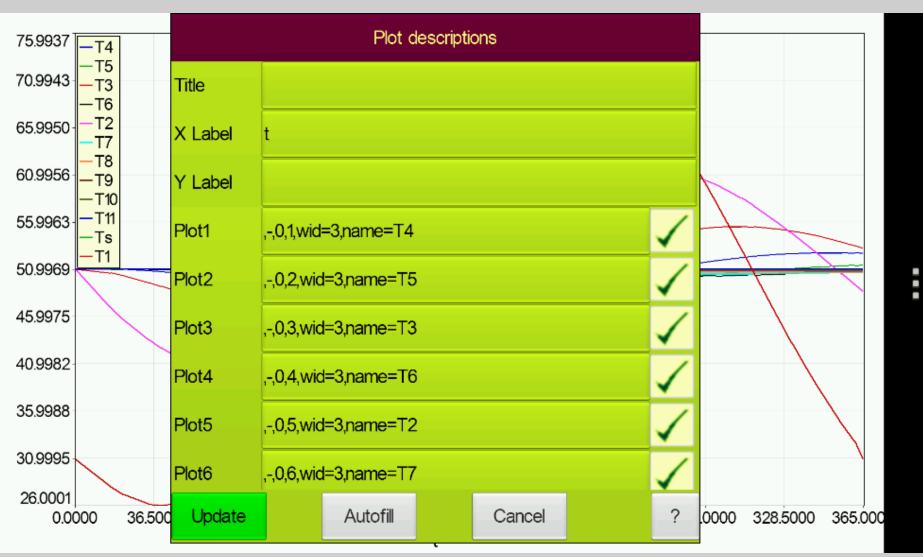


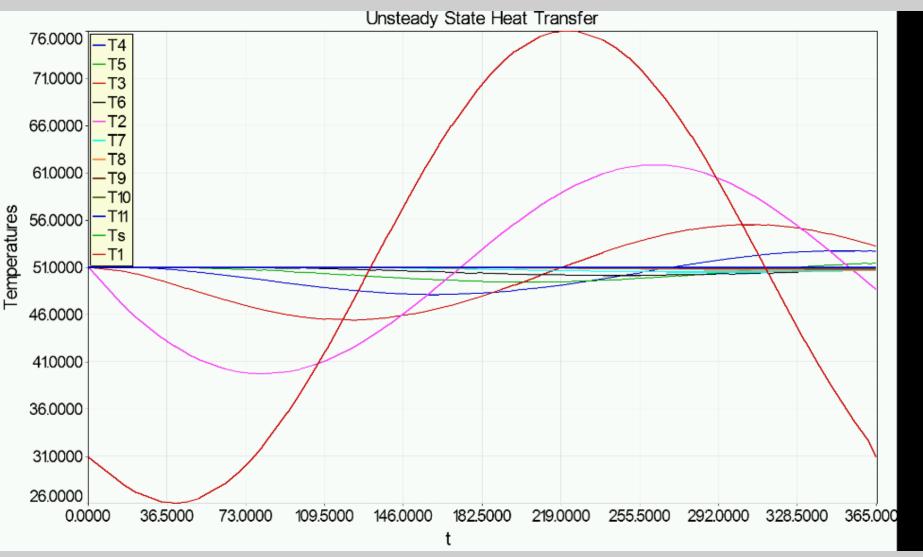




















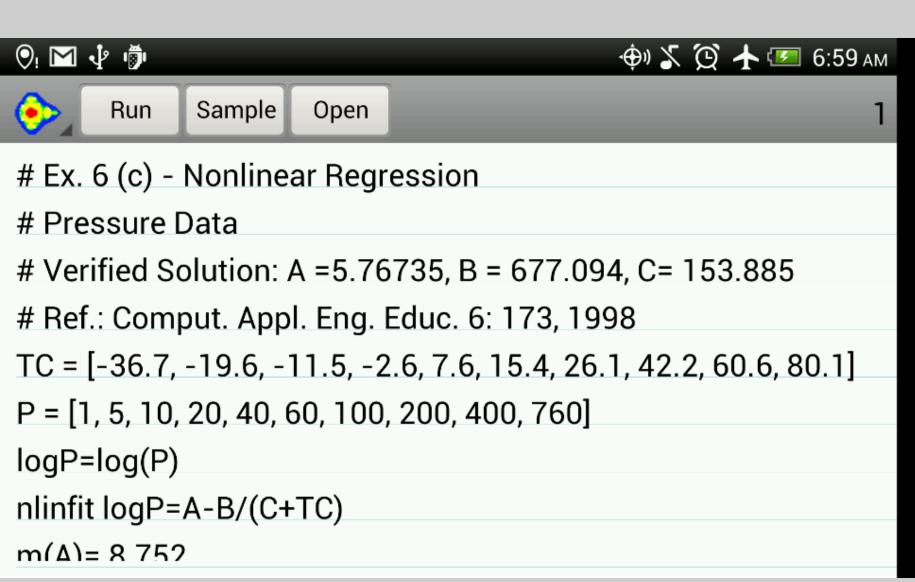






Ex. 6 (c) - Nonlinear Regression
Pressure Data

Ex. 7 - ODE System
Heat Exchange











POLYMATH Report

REG

Nonlinear Regression (L-M)

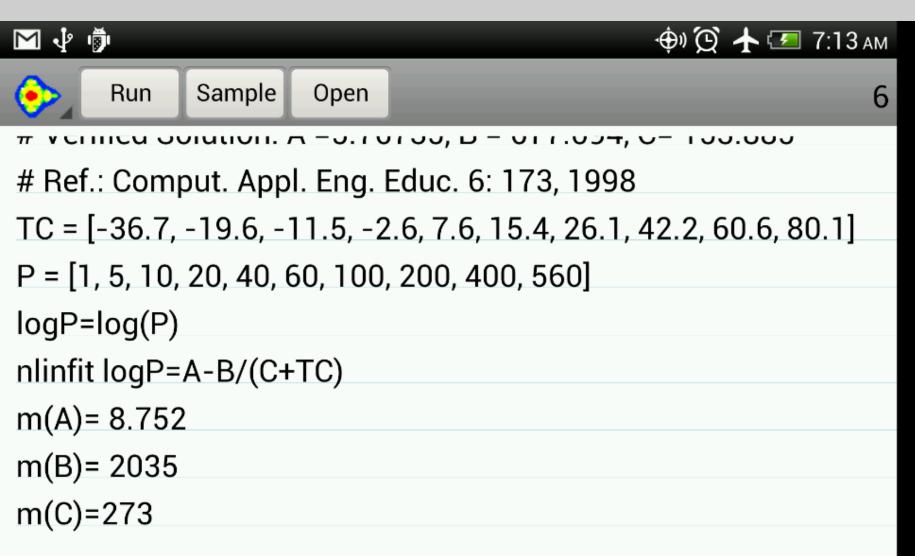
2013-Jun-15

Model: logP = A-B/(C+TC)

Variable	Initial guess	Value	95% confidence		
Α	8.752	5.76735	0.152084		
В	2035	677.094	48.1591		
С	273	153.885	5.68709		

R^2	R^2adj	Rmsd	Variance		
0.9996879	0.9995987	0.0047228	0.0003186		

Source data points and calculated data points









POLYMATH Report

REG

Nonlinear Regression (L-M)

2013-Jun-14

Model: logP = A-B/(C+TC)

Variable	Initial guess	Value	95% confidence		
Α	8.752	5.24952	0.021573		
В	2035	533.906	3.14521		
С	273	137.924	0.75135		

R^2	R^2adj	Rmsd	Variance		
0.9988048	0.9984633	0.0090329	0.0011656		

Source data points and calculated data points







Steady State Material Balances



Molar Volume and Compress... Van Der Waals



Three Phase Equilib.

Ex. 4 - Single NLE

Terminal Velocity

Ex. 5 - NLE System

Reaction Equilibrium

Ex. 6 (a) - Fitting Polynomials

Pressure Data







🐤 Polymath Sample Programs



Ex. 6 (b) - Linear Regression
Pressure Data



Ex. 6 (c) - Nonlinear Regression
Pressure Data



Ex. 7 - ODE System Heat Exchange



Ex. 8- Boundary Value ODE System
Diffusion with Reaction



Ex. 9 - ODE System

Reversible Reaction in a PBR



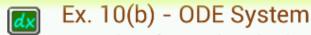
Ex. 10(a) - ODE System

Dynamics of Heated Tank-Open loop

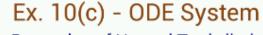




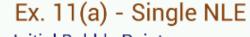
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Dynamics of Heated Tank-Closed loop



Dynamics of Heated Tank-limits on energy input



Initial Bubble Point.



Binary Batch Distillation

Ex. 12 - Single Partial Diff. Eq.

Unsteady State Heat Conduction.

Ex. 13 - Nonlinear Regression

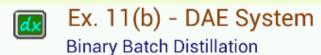
Catalytic Reforming Reac.







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Ex. 14(a) - Multi-Linear Regression
Heat of Hardening

Ex. 14(b) - Multi-Linear Regression via origin
Heat of Hardening

Ex. 15 - Linear Eqs. Biological Reactors







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Ex. 17 - NLE System
Combustion of Propane

Ex. 18 - NLE System
Complex Chemical Equilibrium

Ex. 19 - Consecutive calculations
Gas pressure from SRK equation of state

Ex. 20 - Consecutive calculations
Physical property calculator for liquid CO2