Sequential Calculations with POLYMATH and Excel, Parametric Studies with Excel

These calculations do not require the use of a special numerical technique. The model equations can be written one after another. On the left hand side a variable name appears (the output variable) and the right hand side contains a constant or an expression that may include constants and previously defined variables. Such equations are usually called "explicit" equations.

Typical examples to such calculations involve the solution of cubic equations of state for the compressibility factor for specified value of the temperature T and pressure P.

Molar Volume and Compressibility Factor from Redlich-Kwong Equation

The Redlich-Kwong Equation can be written in terms of the compressibility factor:

$$f(z) = z^3 - z^2 - qz - r = 0$$

$$r = A^2 B$$

$$P_R = P/P_c; \quad T_R = T/T_c$$

$$q = B^2 + B - A^2$$

$$A^2 = 0.42747\left(\frac{P_R}{T_R^{5/2}}\right)$$

$$B = 0.8664\left(\frac{P_R}{T_R}\right)$$

P – pressure in atm
V – molar volume in liters/g-mol
T – temperature in K
R – gas constant (R = 0.08206 (atm·liter/g-mol·K))
T_c – critical temperature in K
P_c – critical pressure in atm

Analytical Solution of the Cubic Redlich-Kwong Equation

The implicit equation for z can be solved analytically for three roots. Considering only the real roots, first the parameter C is calculated:

$$C = \left(\frac{f}{3}\right)^3 + \left(\frac{g}{2}\right)^2$$

where

$$f = \frac{-3q - 1}{3}$$

$$g = \frac{-27r - 9q - 2}{27}$$

If $C>0$ there is one real solution for z:

$$z = D + E + 1/3$$

where

$$D = (-g/2 + \sqrt{C})^{1/3}$$

$$E = (-g/2 - \sqrt{C})^{1/3}$$

After calculating z the molar volume can be calculated:

$$V = zRT/P$$

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If $C<0$ there are three real solution for z:

$$z_k = 2\sqrt{\frac{-f}{3}}\cos\left[\left(\frac{\phi}{3}\right) + \frac{2\pi(k-1)}{3}\right] + \frac{1}{3} \quad k = 1, 2, 3$$

where

$$\phi = a\cos\sqrt{\frac{g^2/4}{(-f^3)/27}}$$

After calculating z the molar volume can be calculated:

$$V = zRT/P$$

Redlich-Kwong Equation Solution Assignment

(a) Use **POLYMATH** to calculate the volume of steam (critical temperature is T_c = 647.4 K and critical pressure is P_c = 218.3 atm) at **T_r = 1.0 and P_r = 1.2**. Compare your result with the value obtained from a physical property data base (V = 0.052456 L/g-mol). Also complete the calculation for T_r = 3.0 and P_r = 10 (V = 0.0837 L/g-mol). Carry out both calculations only if the parameter $C > 0$.

(b) Calculate the compressibility factor and the molar volume of steam using **Excel** for the reduced temperatures and reduced pressures listed in following Table. Prepare a **table and a plot** of the compressibility factor versus P_r and T_r as well as a table and a plot of the molar volume versus pressure and T_r. The pressure and the volume should be in a logarithmic scale in the second plot.

Redlich-Kwong Equation Solution Assignment – Parameter Values

P_r	P_r	P_r	P_r	P_r	T_r
0.1	2	4	6	8	1
0.2	2.2	4.2	6.2	8.2	1.2
0.4	2.4	4.4	6.4	8.4	1.5
0.6	2.6	4.6	6.6	8.6	2.0
0.8	2.8	4.8	6.8	8.8	3.0
1	3	5	7	9	
1.2	3.2	5.2	7.2	9.2	
1.4	3.4	5.4	7.4	9.4	
1.6	3.6	5.6	7.6	9.6	
1.8	3.8	5.8	7.8	9.8	
				10	

Redlich-Kwong Equation Assignment – POLYMATH Code

Line	Equation, # Comment
1	R = 0.08206 # Gas constant (L-atm/g-mol-K)
2	Tc = 647.4 # Critical temperature (K)
3	Pc = 218.3 # Critical pressure (atm)
4	a = 0.42747 * R ^ 2 * Tc ^ (5 / 2) / Pc # Eq.(4-2), RK equation constant
5	b = 0.08664 * R * Tc / Pc # Eq.(4-3),RK equation constant
6	Pr = 1.2 # Reduced pressure (dimensionless
7	Tr = 1 # Reduced temperature (dimensionles
8	r = Asqr * B # Eq.(4-6)
9	q = B ^ 2 + B - Asqr # Eq.(4-7)
10	Asqr = 0.42747 * Pr / (Tr ^ 2.5) # Eq.(4-8)
11	B = 0.08664 * Pr / Tr # Eq.(4-9)
12	C = (f/3) ^ 3 + (g / 2) ^ 2 # Eq.(4-10)
13	f = (-3 * q - 1) / 3 # Eq.(4-11)
14	g = (-27 * r - 9 * q - 2) / 27 # Eq.(4-12)
15	z = If (C > 0) Then (D + E + 1 / 3) Else (0) # Eq.(4-13), Compressibility factor
16	D = If (C > 0) Then ((-g / 2 + sqrt(C)) ^ (1 / 3)) Else (0) # Eq.(4-14)
17	E1 = If (C > 0) Then (-g / 2 - sqrt(C)) Else (0) # Eq.(4-15)
18	E = If (C > 0) Then ((sign(E1) * (abs(E1)) ^ (1 / 3))) Else (0) # Eq.(4-15)
19	P = Pr * Pc # Pressure (atm)
20	T = Tr * Tc # Temperature (K)
21	V = z * R * T / P # Molar volume (L/g-mol)

Note: Row numbers are not part of the code

marks optional comments

Polymath reorders equations

Redlich-Kwong Equation Assignment – POLYMATH Solution

Calculated values of explicit variables

	Variable	Value
1	a	140.6199
2	Asqr	0.512964
3	b	0.0210848
4	B	0.103968
5	C	1.719E-05
6	D	0.1140662
7	E	-0.1895195
8	E1	-0.0068071
9	f	0.0648533
10	g	0.005323
11	P	261.96
12	Pc	218.3
13	Pr	1.2
14	q	-0.3981867
15	R	0.08206
16	r	0.0533318
17	T	647.4
18	Tc	647.4
19	Tr	1.
20	V	0.0522982
21	z	0.25788

Compare your result with the value obtained from a physical property data base (V = 0.052456 L/g-mol).

Redlich-Kwong Equation Assignment – Export to Excel

Microsoft Excel - P4-1B1

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Documentation

	A	B	C	D	E
1	POLYM.				
2		Variable	Value		Polymath Equation
3	Explicit Eqs	R	=0.08206		R=0.08206
4		Tc	=647.4		Tc=647.4
5		Pc	=218.3		Pc=218.3
6		a	=(((0.42747 * (C3 ^ 2)) * (C4 ^ (5 / 2))) / C5)		a=0.42747 * R ^ 2 * Tc ^ (5 / 2) / Pc
7		b	=(((0.08664 * C3) * C4) / C5)		b=0.08664 * R * Tc / Pc
8		Pr	=1.2		Pr=1.2
9		Tr	=1		Tr=1
10		r	=(C12 * C13)		r=Asqr * B
11		q	=(((C13 ^ 2) + C13) - C12)		q=B ^ 2 + B - Asqr
12		Asqr	=((0.42747 * C8) / (C9 ^ 2.5))		Asqr=0.42747 * Pr / (Tr ^ 2.5)
13		B	=((0.08664 * C8) / C9)		B=0.08664 * Pr / Tr
14		C	=(((C15 / 3) ^ 3) + ((C16 / 2) ^ 2))		C=(f/3) ^ 3 + (g / 2) ^ 2
15		f	=(((-3 * C11) - 1) / 3)		f=(-3 * q - 1) / 3
16		g	=((((-27 * C10) - (9 * C11)) - 2) / 27)		g=(-27 * r - 9 * q - 2) / 27
17		z	=IF((C14 > 0),((C18 + C20) + (1 / 3)),0)		z=If (C > 0) Then (D + E + 1 / 3) Else (0)
18		D	=IF((C14 > 0),(((0 - (C16 / 2)) + SQRT(C14)) ^ (1 / 3)),0)		D=If (C > 0) Then ((-g / 2 + sqrt(C)) ^ (1 / 3)) Else (0)
19		E1	=IF((C14 > 0),((0 - (C16 / 2)) - SQRT(C14)),0)		E1=If (C > 0) Then (-g / 2 - sqrt(C)) Else (0)
20		E	=IF((C14 > 0),(SIGN(C19) * (ABS(C19) ^ (1 / 3))),0)		E=If (C > 0) Then ((sign(E1) * (abs(E1)) ^ (1 / 3))) Else (0)
21		P	=(C8 * C5)		P=Pr * Pc
22		T	=(C9 * C4)		T=Tr * Tc
23		V	=(((C17 * C3) * C22) / C21)		V=z * R * T / P
24					

Excel formulas

Redlich-Kwong Equation Assignment – Export to Excel

Documentation

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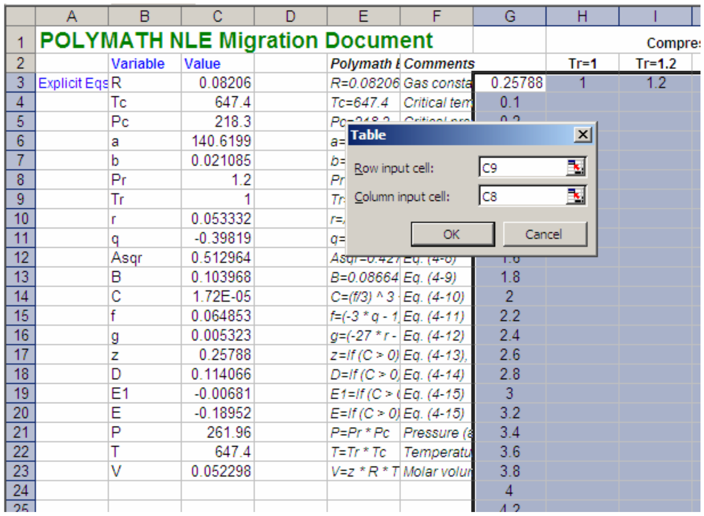
	A	B	C	D	E	F
1	POLYMATH NLE Migration Document					
2		Variable	Value		Polymath Equation	Comments
3	Explici	R	0.08206		R=0.08206	Gas constant (L-atm/g-mol-K)
4		Tc	647.4		Tc=647.4	Critical temperature (K)
5		Pc	218.3		Pc=218.3	Critical pressure (atm)
6		a	140.6198623		a=0.42747 * R ^ 2 * Tc ^ (5 / 2) / Pc	Eq. (4-2), RK equation constant
7		b	0.021084772		b=0.08664 * R * Tc / Pc	Eq. (4-3),RK equation constant
8		Pr	1.2		Pr=1.2	Reduced pressure (dimensionless)
9		Tr	1		Tr=1	Reduced temperature (dimensionless
10		r	0.053331841		r=Asqr * B	Eq. (4-6)
11		q	-0.398186655		q=B ^ 2 + B - Asqr	Eq. (4-7)
12		Asqr	0.512964		Asqr=0.42747 * Pr / (Tr ^ 2.5)	Eq. (4-8)
13		B	0.103968		B=0.08664 * Pr / Tr	Eq. (4-9)
14		C	1.71861E-05		C=(f/3) ^ 3 + (g / 2) ^ 2	Eq. (4-10)
15		f	0.064853322		f=(-3 * q - 1) / 3	Eq. (4-11)
16		g	0.00532297		g=(-27 * r - 9 * q - 2) / 27	Eq. (4-12)
17		z	0.257880011		z=If (C > 0) Then (D + E + 1 / 3) Else (0)	Eq. (4-13), Compressibility factor (dim
18		D	0.114066207		D=If (C > 0) Then ((-g / 2 + sqrt(C)) ^ (1 / 3)) Else (0)	Eq. (4-14)
19		E1	-0.006807097		E1=If (C > 0) Then (-g / 2 - sqrt(C)) Else (0)	Eq. (4-15)
20		E	-0.18951953		E=If (C > 0) Then ((sign(E1) * (abs(E1)) ^ (1 / 3))) Else (0)	Eq. (4-15)
21		P	261.96		P=Pr * Pc	Pressure (atm)
22		T	647.4		T=Tr * Tc	Temperature (K)
23		V	0.05229822		V=z * R * T / P	Molar volume (L/g-mol)
24						

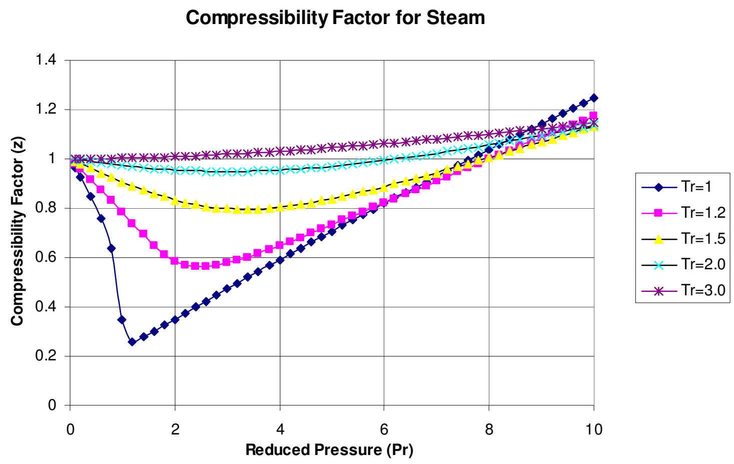
Redlich-Kwong Equation Assignment – Parametric Study Using Excel Table



Redlich-Kwong Equation Assignment – z versus T_R and P_R

G	H	I	J	K	L
	Compressibility Factor (z)				
	Tr=1	Tr=1.2	Tr=1.5	Tr=2.0	Tr=3.0
0.25788	1	1.2	1.5	2	3
0.1	0.965162	0.979972	0.990293	0.996817	1.000162
0.2	0.928637	0.959637	0.980652	0.993718	1.000356
0.4	0.849068	0.918005	0.961605	0.987783	1.000842
0.6	0.756568	0.875036	0.942949	0.982211	1.001457
0.8	0.638741	0.830724	0.924788	0.97702	1.002201
1	0.346664	0.785203	0.907245	0.972226	1.003072
1.2	0.25788	0.73893	0.890458	0.967843	1.00407
1.4	0.276763	0.692999	0.87458	0.963885	1.005193
1.6	0.299892	0.649616	0.859774	0.960365	1.006441
1.8	0.324267	0.61227	0.84621	0.957292	1.007811
2	0.349051	0.584569	0.834049	0.954675	1.009304
2.2	0.373921	0.567974	0.823438	0.952519	1.010916
2.4	0.398736	0.5612	0.814496	0.95083	1.012648
2.6	0.423428	0.561787	0.807302	0.949609	1.014495
2.8	0.447965	0.567497	0.801891	0.948854	1.016458
3	0.472333	0.576704	0.798254	0.948563	1.018534
3.2	0.496528	0.588318	0.796335	0.948731	1.020721
3.4	0.52055	0.601614	0.796048	0.949351	1.023017
3.6	0.544403	0.616107	0.797279	0.950413	1.02542
3.8	0.568092	0.631467	0.799901	0.951906	1.027928
4	0.591623	0.647463	0.803779	0.953819	1.030539
4.2	0.615002	0.663931	0.808781	0.956138	1.03325
4.4	0.638236	0.680752	0.814781	0.958848	1.03606

Redlich-Kwong Equation Assignment – z versus T_R and P_R



Redlich-Kwong Equation Assignment – V versus T_R and P