

VLE Calculation using Excel Spreadsheet

Suppose you have a mixture of hydrocarbons in the inlet stream. You want to find the fraction of the stream that is vapor and the mole fraction of each chemical in the vapor and liquid streams. Table 1 shows the flow rates and K-values at 180 °F and 70 psia, using a basis of one mole per unit of time.

Table 1. Mole Fractions and K-values for Vapor–Liquid Example

	Mole Fraction	Phase Equilibrium K-value
Propane	0.1	6.8
n-Butane	0.3	2.2
n-Pentane	0.4	0.8
n-Octane	0.2	0.052
	1	

To solve this problem, prepare the spreadsheet as shown in Table 2

Table 2. Spreadsheet Calculation

	A	B	C	D	E	F	G	H
1				$v = 0.425837$				
2			Phase					
3			Equilibrium	term1 =	term2 =	Ratio =		
4		z_i	K-value	$(K_i - 1)z_i$	$(K_i - 1)v + 1$	term1/term2	x_i	y_i
5	Propane	0.1	6.8	0.58	3.4699	0.1672	0.0288	0.1960
6	n-Butane	0.3	2.2	0.36	1.5110	0.2383	0.1985	0.4368
7	n-Pentane	0.4	0.8	-0.08	0.9148	-0.0874	0.4372	0.3498
8	n-Octane	0.2	0.052	-0.1896	0.5963	-0.3180	0.3354	0.0174
		1			$f(v) = 8.2719E-07$		0.9999996	1.0000005

Step 1 ‘Term1’ is the numerator in Eq.

$$\sum_{i=1}^{NCOMP} \frac{(K_i - 1)z_i}{1 + (K_i - 1)v'} = 0$$

and ‘term2’ is the denominator, and these are calculated in columns D and E.

Step 2 The ratios of term1 over term2 are calculated and put into column F; this column is summed in cell F9, which represents the equation

$$\sum_{i=1}^{NCOMP} \frac{(K_i - 1)z_i}{1 + (K_i - 1)v'} = 0$$

Step 3 You can then use Goal Seek to make the Rachford–Rice equation (cell F9) zero by changing the fraction of the feed that is vapor (cell D1), giving the result shown. Once you find the fraction vapor, the mole fractions in the two phases are easy to calculate using equations

$$y_i = K_i x_i$$

and

$$x_i = \frac{z_i}{1 + (K_i - 1)v'}$$

Reference:

Bruce A. Finlayson, *Introduction to Chemical Engineering Computing*, John Wiley and Sons, 2006 Edition, pp 26-29.