Example:

For the production of ethanol from ethylene and water at 250 °C and 35 bar with initial ratio $n_{0H_2O}/n_{0C_2H_4} = 5$, estimate the equilibrium conversion without assuming ideal gas behavior. Assume in your analysis ideal solution behavior.

$$C_2H_4(g) + H_2O(g) \rightarrow C_2H_5OH(g)$$

Solution:

Basis: 5 moles initially for water ➔ 1 mole of ethylene.

At equilibrium:

$$K\left(\frac{P}{P^o}\right)^{-\nu} = \prod_i \left(y_i \hat{\phi}_i\right)^{\nu_i}$$

and by assuming an ideal solution, the equation simplifies to:

$$K\left(\frac{P}{P^o}\right)^{-\nu} = \prod_i \left(y_i \phi_i\right)^{\nu_i}$$

At 250 °C the equilibrium constant, $K = 10.02 * 10^{-3}$ (see example 13.4). Substituting in the equilibrium relation:

$$10.02\times10^{-3}\left(\frac{35}{1}\right)^{-(-1)} = 0.3507 = \frac{y_3\phi_3}{y_1\phi_1 y_2\phi_2}$$

We need to evaluate ϕ_i using an appropriate correlation such as Lee/Kesler:

Species	ω_i	T_{ri}	P_{ri}	ϕ_i
C_2H_4 (1)	0.087	1.853	0.694	0.977
H_2O (2)	0.345	0.808	0.159	0.887
C_2H_5OH (3)	0.645	1.018	0.569	0.827

Substituting in the previous relation:

$$0.3507 = \frac{0.827\ y_3}{(0.977)(0.887)y_1 y_2}$$

Simplifying:

$$\frac{y_3}{y_1 y_2} = 0.3675$$

Recall, $$y_i = \frac{n_i}{n} = \frac{n_{i0} + \nu_i \varepsilon}{n_0 + \nu \varepsilon}$$

Therefore: $y_1 = \frac{1-\varepsilon_e}{6-\varepsilon_e}$, $y_2 = \frac{5-\varepsilon_e}{6-\varepsilon_e}$ and $y_3 = \frac{\varepsilon_e}{6-\varepsilon_e}$.

Substituting:

$$\frac{\varepsilon_e(6-\varepsilon_e)}{(5-\varepsilon_e)(1-\varepsilon_e)} = 0.367$$

Simplifying:

$$1.367\varepsilon_e^2 - 8.202\varepsilon_e + 1.835 = 0$$

$$\Rightarrow \varepsilon_e = 0.233 \text{ or } 5.767$$

Note: $\varepsilon_e = \frac{n-n_0}{\nu} = \frac{n-6}{-1} = 6-n$ which cannot exceed 1. Therefore, $\boldsymbol{\varepsilon_e = 0.233}$.