Equilibrium conversion of Multiple Reactions

13.33. The feed gas to a methanol synthesis reactor is composed of 75-mol-% H_2, 15-mol-% CO, 5-mol-% CO_2, and 5-mol-% N_2. The system comes to equilibrium at 550 K and 100 bar with respect to the following reactions:

$$2H_2(g) + CO(g) \rightarrow CH_3OH(g)$$

$$H_2(g) + CO_2(g) \rightarrow CO(g) + H_2O(g)$$

Assuming ideal gases, determine the composition of the equilibrium mixture.

Solution

Basis 1 mole of feed:

$\Rightarrow n_{o_{H_2}} = 0.75$ (mole)

$n_{o_{CO}} = 0.15$ "

$n_{o_{CO_2}} = 0.05$ (mole)

$n_{o_{N_2}} = 0.05$ "

$n_{o_{CH_3OH}} = n_{o_{H_2O}} = 0$

$(\gamma)_1 = 1 - 2 - 1 = -2$

$(\gamma)_2 = 1 + 1 - 1 - 1 = 0$

$K_1 = 6.749 * 10^{-4}$ (do it yourself)

$K_2 = 0.01726$ (")

i =	H_2	CO	CO_2	CH_3OH	H_2O	
j						γ_j
1	-2	-1	0	1	0	-2
2	-1	1	-1	0	1	0

$$y_i = \frac{n_{i0} + \sum_j \nu_{ij} \varepsilon_j}{n_0 + \sum_j \nu_j \varepsilon_j}$$

$$y_{H_2} = \frac{0.75 - 2\varepsilon_1 - 1\varepsilon_2}{1 - 2\varepsilon_1 + 0\varepsilon_2} = \frac{0.75 - 2\varepsilon_1 - \varepsilon_2}{1 - 2\varepsilon_1}$$

$$y_{CO} = \frac{0.15 - \varepsilon_1 + \varepsilon_2}{1 - 2\varepsilon_1}$$

$$y_{CO_2} = \frac{0.05 - \varepsilon_2}{1 - 2\varepsilon_1}$$

$$y_{CH_3OH} = \frac{\varepsilon_1}{1 - 2\varepsilon_1}$$

$$y_{H_2O} = \frac{\varepsilon_2}{1 - 2\varepsilon_1}$$

Equilibrium:

$$K_j \left(\frac{P}{P_0}\right)^{-\nu_j} = \prod_i \left(y_{ij}\right)^{\nu_i}$$

$$K_1 \left(\frac{P}{P_0}\right)^{+2} = \frac{y_{CH_3OH}}{y_{CO}\ y_{H_2}^2}$$

$$K_2 \left(\frac{P}{P_0}\right)^{0} = \frac{y_{CO}\ y_{H_2O}}{y_{H_2}\ y_{CO_2}}$$

substitute

$$6.749 * 10^{-4} \left(\frac{100}{1}\right)^2 = \frac{\dfrac{\varepsilon_1}{(1-2\varepsilon_1)}}{\dfrac{(0.15-\varepsilon_1+\varepsilon_2)}{(1-2\varepsilon_1)}\left(\dfrac{0.75-2\varepsilon_1-\varepsilon_2}{1-2\varepsilon_1}\right)^2}$$

$$0.01726\ (1) = \frac{\dfrac{(0.15-\varepsilon_1+\varepsilon_2)}{(1-2\varepsilon_1)}\ \dfrac{\varepsilon_2}{(1-2\varepsilon_1)}}{\dfrac{(0.75-2\varepsilon_1-\varepsilon_2)}{(1-2\varepsilon_1)}\ \dfrac{(0.05-\varepsilon_2)}{(1-2\varepsilon_1)}}$$

$$6.749 = \frac{\varepsilon_1\ (1-2\varepsilon_1)^2}{(0.75-2\varepsilon_1-\varepsilon_2)^2\ (0.15-\varepsilon_1+\varepsilon_2)} \quad (1)$$

$$0.01726 = \frac{(0.15-\varepsilon_1+\varepsilon_2)(\varepsilon_2)}{(0.75-2\varepsilon_1-\varepsilon_2)(0.05-\varepsilon_2)} \quad (2)$$

We have two equations with two unknowns ε_1 & ε_2. Solve by trail and error

$$\Rightarrow \quad \varepsilon_1 = 0.1186 \quad \& \quad \varepsilon_2 = 0.0089$$

$$\Rightarrow y_{H_2} = 0.6606 \qquad y_{CO} = 0.0528 \qquad y_{CO_2} = 0.0655$$

$$y_{CH_3OH} = 0.1555 \qquad y_{H_2O} = 0.0116 \qquad y_{N_2} = 0.0655$$

$$\uparrow$$

$$= 1 - \sum_i y_i$$