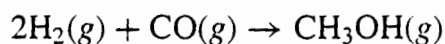


# Equilibrium Conversion of Multiple Reactions

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:



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

## Solution

Basis 1 mole of feed:

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

$$n_{O_{CO}} = 0.15 \text{ ''}$$

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

$$n_{O_{CO_2}} = 0.05 \text{ (mole)}$$

$$n_{O_{N_2}} = 0.05 \text{ ''}$$

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

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

$$K_1 = 6.749 \times 10^{-4}$$

(do it yourself)

$$K_2 = 0.01726$$

( " )

$i =$	$H_2$	$CO$	$CO_2$	$CH_3OH$	$H_2O$	
$j$						$\gamma_j$
1	-2	-1	0	1	0	-2
2	-1	1	-1	0	1	0

$$y_i = \frac{n_{i0} + \sum_j \gamma_{ij} \epsilon_j}{n_0 + \sum_j \gamma_j \epsilon_j}$$

$$y_{H_2} = \frac{0.75 - 2\epsilon_1 - 1\epsilon_2}{1 - 2\epsilon_1 + 0\epsilon_2} = \frac{0.75 - 2\epsilon_1 - \epsilon_2}{1 - 2\epsilon_1}$$

$$y_{CO} = \frac{0.15 - \epsilon_1 + \epsilon_2}{1 - 2\epsilon_1}$$

$$y_{CO_2} = \frac{0.05 - \epsilon_2}{1 - 2\epsilon_1}$$

$$y_{CH_3OH} = \frac{\epsilon_1}{1 - 2\epsilon_1}$$

$$y_{H_2O} = \frac{\epsilon_2}{1 - 2\epsilon_1}$$

Equilibrium:

(3)

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

$$K_1 \left( \frac{P}{P_0} \right)^{+2} = \frac{y_{\text{CA}_3\text{O}_4}}{y_{\text{CO}} y_{\text{H}_2}^2}$$

$$K_2 \left( \frac{P}{P_0} \right)^0 = \frac{y_{\text{CO}} y_{\text{H}_2\text{O}}}{y_{\text{A}_2} y_{\text{CO}_2}}$$

substitute

$$6.749 \times 10^{-4} \left( \frac{100}{1} \right)^2 = \frac{\frac{\epsilon_1}{(1-2\epsilon_1)}}{\frac{(0.15 - \epsilon_1 + \epsilon_2)}{(1-2\epsilon_1)} \left( \frac{0.75 - 2\epsilon_1 - \epsilon_2}{1-2\epsilon_1} \right)^2}$$
$$0.01726 (1) = \frac{\frac{\epsilon_1}{(1-2\epsilon_1)}}{\frac{(0.15 - \epsilon_1 + \epsilon_2)}{(1-2\epsilon_1)} \frac{\epsilon_2}{(1-2\epsilon_1)} \frac{(0.75 - 2\epsilon_1 - \epsilon_2)}{(1-2\epsilon_1)}}$$

$$6.749 = \frac{\epsilon_1 (1-2\epsilon_1)^2}{(0.75 - 2\epsilon_1 - \epsilon_2)^2 (0.15 - \epsilon_1 + \epsilon_2)} \quad (1)$$

$$0.01726 = \frac{(0.15 - \epsilon_1 + \epsilon_2)(\epsilon_2)}{(0.75 - 2\epsilon_1 - \epsilon_2)(0.05 - \epsilon_2)} \quad (2)$$

We have two equations with two unknowns <sup>4</sup>  
 $\epsilon_1$  &  $\epsilon_2$ . Solve by trial and error

$$\Rightarrow \epsilon_1 = 0.1186 \quad \& \quad \epsilon_2 = 0.0089$$

$$\Rightarrow y_{H_2} = 0.6606$$

$$y_{CO} = 0.0528$$

$$y_{CO_2} = 0.0655$$

$$y_{CH_3OH} = 0.1555$$

$$y_{H_2O} = 0.0116$$

$$y_{N_2} = 0.0655$$

↑

$$= 1 - \sum_i y_i$$