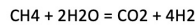
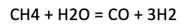


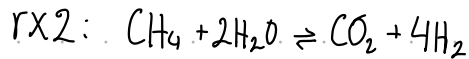
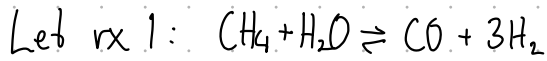
Exercise 13

1. Reaction Equilibrium

Determine the expressions for the two equilibrium constants of the system characterized by the two chemical reactions:



Assume ideal gas.



And the extent of each reaction be ξ_1 for rx 1 and ξ_2 for rx 2.

The reactions are linearly independent, so we already have linearly independent system.

We did the same problem in the lectures, and used $n_{\text{CH}_4,0} = 1$ and

$n_{\text{H}_2\text{O},0} = 2$, so I will do the same for simplicity.

Component	CH_4	H_2O	CO	CO_2	H_2
V_1	-1	-1	1	0	3
V_2	-1	-2	0	1	4
$n_{i,0}$	1	2	0	0	0
n_i	$1 - \xi_1 - \xi_2$	$2 - \xi_1 - 2\xi_2$	ξ_1	ξ_2	$3\xi_1 + 4\xi_2$

We have that the total number of moles in the system is given by: $n = \sum n_i = (1 - \xi_1 - \xi_2) + (2 - \xi_1 - 2\xi_2) + \xi_1 + \xi_2 + (3\xi_1 + 4\xi_2)$

$$n = 3 + 2\xi_1 + 2\xi_2$$

Using that $y_i = \frac{n_i}{n}$, we get: $y_{\text{CH}_4} = \frac{1 - \xi_1 - \xi_2}{3 + 2\xi_1 + 2\xi_2}$

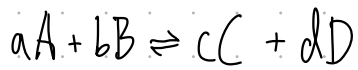
$$y_{\text{H}_2\text{O}} = \frac{2 - \xi_1 - 2\xi_2}{3 + 2\xi_1 + 2\xi_2}$$

$$y_{\text{CO}} = \frac{\xi_1}{3 + 2\xi_1 + 2\xi_2}$$

$$y_{\text{CO}_2} = \frac{\xi_2}{3 + 2\xi_1 + 2\xi_2}$$

$$y_{\text{H}_2} = \frac{3\xi_1 + 4\xi_2}{3 + 2\xi_1 + 2\xi_2}$$

In the lectures, it was shown that for the general reaction



by assuming ideal gas, the equilibrium constant is given by:

$$K \stackrel{ig}{=} \frac{y_C^c \cdot y_D^d}{y_A^a \cdot y_B^b} \cdot \left(\frac{P}{P^0} \right)^{c+d-a-b}$$

Applying this to the two reactions, the equilibrium constants can be found:

$$K_1 = \frac{y_{CO} \cdot y_{H_2}^3}{y_{CH_4} \cdot y_{H_2O}} \cdot \left(\frac{P}{P^0} \right)^{1+3-1-1}$$

$$K_2 = \frac{y_{CO_2} \cdot y_{H_2}^4}{y_{CH_4} \cdot y_{H_2O}^2} \cdot \left(\frac{P}{P^0} \right)^{1+4-1-2}$$

$$K_1 = \frac{\frac{\xi_1}{(3+2\xi_1+2\xi_2)} \cdot \frac{(3\xi_1+4\xi_2)^3}{(3+2\xi_1+2\xi_2)}}{\frac{(1-\xi_1-\xi_2)}{(3+2\xi_1+2\xi_2)} \cdot \frac{(2-\xi_1-2\xi_2)}{(3+2\xi_1+2\xi_2)}} \cdot \left(\frac{P}{P^0} \right)^2$$

$$K_2 = \frac{\frac{\xi_2}{(3+2\xi_1+2\xi_2)} \cdot \frac{(3\xi_1+4\xi_2)^4}{(3+2\xi_1+2\xi_2)}}{\frac{(1-\xi_1-\xi_2)}{(3+2\xi_1+2\xi_2)} \cdot \frac{(2-\xi_1-2\xi_2)^2}{(3+2\xi_1+2\xi_2)}} \cdot \left(\frac{P}{P^0} \right)^2$$

$$K_1 = \frac{\xi_1(3\xi_1+4\xi_2)^3}{(1-\xi_1-\xi_2)(2-\xi_1-2\xi_2)(3+2\xi_1+2\xi_2)^2} \cdot \left(\frac{P}{P^0} \right)^2$$

$$K_2 = \frac{\xi_2(3\xi_1+4\xi_2)^4}{(1-\xi_1-\xi_2)(2-\xi_1-2\xi_2)^2(3+2\xi_1+2\xi_2)^2} \cdot \left(\frac{P}{P^0} \right)^2$$