REB, The Course
Class 2, Activity 2 Solution

The charge to a reactor consisted of 66 mol H_2 and 34 mol CO. Reactions (1) through (6) occurred, after which 40% of the CO had been converted. The final ratio of H2 to CO was 1.5, and the selectivity for methanol over carbon dioxide was 8.3. Calculate the final molar amount of each reagent in the system.

$$CO + 2H_2 \rightleftarrows CH_3OH \tag{1}$$

$$CO_2 + 3H_2 \leftrightarrows CH_3OH + H_2O \tag{2}$$

$$CO + H_2O \leftrightarrows CO_2 + H_2 \tag{3}$$

$$CO + 3H_2 \leftrightarrows CH_4 + H_2O \tag{4}$$

$$CO_2 + 4H_2 \leftrightarrows CH_4 + 2H_2O \tag{5}$$

$$CH_4 + H_2O \leftrightarrows CH_3OH + H_2 \tag{6}$$

Generate a complete, independent subset of the reactions starting with the transpose of the stoichiometric coefficient matrix.

$$\boldsymbol{\nu}^T = \begin{bmatrix} -1 & -2 & 1 & 0 & 0 & 0 \\ 0 & -3 & 1 & -1 & 1 & 0 \\ -1 & 1 & 0 & 1 & -1 & 0 \\ -1 & -3 & 0 & 0 & 1 & 1 \\ 0 & -4 & 0 & -1 & 2 & 1 \\ 0 & 1 & 1 & 0 & -1 & -1 \end{bmatrix} \tag{7}$$

The rank of $\boldsymbol{\nu}^T$ is 3, so only three reactions are independent. The rank of a working matrix, $\boldsymbol{W}_1$, that contains only the first two rows of $\boldsymbol{\nu}^T$, equation (8) is 2, so the first two reactions are independent.

$$\boldsymbol{W}_1 = \begin{bmatrix} -1 & -2 & 1 & 0 & 0 & 0 \\ 0 & -3 & 1 & -1 & 1 & 0 \end{bmatrix} \tag{8}$$

The rank of a working matrix, $\boldsymbol{W}_2$, that contains only the first three rows of $\boldsymbol{\nu}^T$, equation (9) is also 2, so the third reaction is not independent.

$$\boldsymbol{W}_2 = \begin{bmatrix} -1 & -2 & 1 & 0 & 0 & 0 \\ 0 & -3 & 1 & -1 & 1 & 0 \\ -1 & 1 & 0 & 1 & -1 & 0 \end{bmatrix} \tag{9}$$

The rank of a working matrix, $\boldsymbol{W}_3$, that contains only the first, second, and fourth rows of $\boldsymbol{\nu}^T$, equation (10) is 3, so reactions (1), (2), and (4) form a complete, independent subset of the reactions.

$$\boldsymbol{W}_3 = \begin{bmatrix} -1 & -2 & 1 & 0 & 0 & 0 \\ 0 & -3 & 1 & -1 & 1 & 0 \\ -1 & -3 & 0 & 0 & 1 & 1 \end{bmatrix} \tag{10}$$

Use the given information to calculate the apparent extents of reaction.

Given: $n_{H_2,0}$ = 66 mol, $n_{CO,0}$ = 34 mol, f_{CO} = 0.4, $x_{H_2/CO}$ = 1.5, and S_{CH_3OH/CO_2} = 8.3

Express the given information in terms of the apparent extents of reaction:

$$f_{CO} = \frac{n_{CO,0} - n_{CO}}{n_{CO,0}} = \frac{n_{CO,0} - \left(n_{CO,0} - \xi_1 - \xi_4\right)}{n_{CO,0}}$$

$$f_{CO} = \frac{\xi_1 + \xi_4}{n_{CO,0}} \tag{11}$$

$$x_{H_2/CO} = \frac{n_{H_2}}{n_{CO}}$$

$$= \tag{12}$$

$$S_{CH_3OH/CO_2} = \frac{n_{CH_3OH}}{n_{CO_2}} = \frac{n_{CH_3OH,0} + \xi_1 + \xi_2}{n_{CO_2,0} - \xi_2}$$

$$S_{CH_3OH/CO_2} = \frac{\xi_1 + \xi_2}{-\xi_2} \tag{13}$$

Solve equations (11) - (13) to get ξ_1 = 4.08 mol, ξ_2 = -0.44 mol, and ξ_3 = 9.52 mol. Use the apparent extents of reaction to calculate the quantities of interest

$$n_{CO} = n_{CO,0} - \xi_1 - \xi_4 = 20.4 \text{ mol}$$

$$n_{H_2} = n_{H_2,0} - 2\xi_1 - 3\xi_2 - 3\xi_4 = 30.6 \text{ mol}$$

$$n_{CH_3OH} = n_{CH_3OH,0} + \xi_1 + \xi_2 = 3.64 \text{ mol}$$

$$n_{CO_2} = n_{CO_2,0} - \xi_2 = 0.44 \text{ mol}$$

$$n_{H_2O} = n_{H_2O,0} + \xi_2 + \xi_4 = 9.08 \text{ mol}$$

$$n_{CH_4} = n_{CH_4,0} + \xi_4 = 9.52 \text{ mol}$$