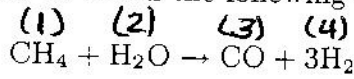


Example 13.1 For a system in which the following reaction occurs,



assume there are present initially 2 mol CH<sub>4</sub>, 1 mol H<sub>2</sub>O, 1 mol CO, and 4 mol H<sub>2</sub>. Determine expressions for the mole fractions  $y_i$  as functions of  $\epsilon$ .

$$y_i = \frac{n_{i0} + \gamma_i \epsilon}{n_0 + \gamma \epsilon}$$

$$n_{10} = 2, \quad n_{20} = 1, \quad n_{30} = 1 \quad \& \quad n_{40} = 4$$

$$\gamma_1 = -1, \quad \gamma_2 = -1, \quad \gamma_3 = +1 \quad \& \quad \gamma_4 = +3$$

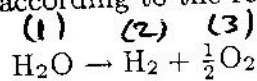
$$\gamma = (-1) + (-1) + (1) + (3) = 2$$

$$n_0 = 2 + 1 + 1 + 4 = 8$$

$$y_1 = \frac{2 + (-1)\epsilon}{8 + 2\epsilon} = \frac{2 - \epsilon}{8 + 2\epsilon}, \quad y_2 = \frac{1 - \epsilon}{8 + 2\epsilon}$$

$$y_3 = \frac{1 + \epsilon}{8 + 2\epsilon}, \quad y_4 = \frac{4 + 3\epsilon}{8 + 2\epsilon}$$

Example 13.2 Consider a vessel which initially contains only  $n_0$  moles of water vapor. If decomposition occurs according to the reaction



$$\gamma = \frac{1}{2}$$

find expressions which relate the number of moles and the mole fraction of each chemical species to the reaction coordinate  $\epsilon$ .

$$n_i = n_{i0} + \sum \gamma_i \epsilon$$

$$n_1 = n_0 - \epsilon$$

$$n_2 = \epsilon$$

$$n_3 = \frac{1}{2} \epsilon$$

$$y_i = \frac{n_{i0} + \gamma_i \epsilon}{n_0 + \gamma \epsilon}$$

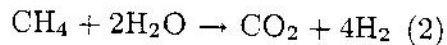
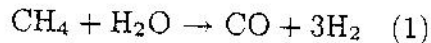
$$y_1 = \frac{n_0 - \epsilon}{n_0 + \frac{1}{2} \epsilon}$$

$$y_2 = \frac{\epsilon}{n_0 + \frac{1}{2} \epsilon}$$

$$y_3 = \frac{\frac{1}{2} \epsilon}{n_0 + \frac{1}{2} \epsilon}$$

for this problem,  $(n_{10} = n_0)$

**Example 13.3** Consider a system in which the following reactions occur:



where the numbers (1) and (2) indicate the value of  $j$ , the reaction index. If there are present initially 2 mol  $\text{CH}_4$  and 3 mol  $\text{H}_2\text{O}$ , determine expressions for the  $y_i$  as functions of  $\varepsilon_1$  and  $\varepsilon_2$ .

**SOLUTION** The stoichiometric numbers  $\nu_{i,j}$  can be arrayed as follows:

| $i =$ | $\text{CH}_4$ | $\text{H}_2\text{O}$ | $\text{CO}$ | $\text{CO}_2$ | $\text{H}_2$ |         |
|-------|---------------|----------------------|-------------|---------------|--------------|---------|
|       |               |                      |             |               |              | $\nu_j$ |
| 1     | -1            | -1                   | 1           | 0             | 3            | 2       |
| 2     | -1            | -2                   | 0           | 1             | 4            | 2       |

Application of Eq. (13.7) now gives

$$y_{\text{CH}_4} = \frac{2 - \varepsilon_1 - \varepsilon_2}{5 + 2\varepsilon_1 + 2\varepsilon_2}$$

$$y_{\text{H}_2\text{O}} = \frac{3 - \varepsilon_1 - 2\varepsilon_2}{5 + 2\varepsilon_1 + 2\varepsilon_2}$$

$$y_{\text{CO}} = \frac{\varepsilon_1}{5 + 2\varepsilon_1 + 2\varepsilon_2}$$

$$y_{\text{CO}_2} = \frac{\varepsilon_2}{5 + 2\varepsilon_1 + 2\varepsilon_2}$$

$$y_{\text{H}_2} = \frac{3\varepsilon_1 + 4\varepsilon_2}{5 + 2\varepsilon_1 + 2\varepsilon_2}$$

The composition of the system is a function of the independent variables  $\varepsilon_1$  and  $\varepsilon_2$ .