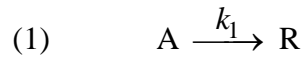


Problem 2-06 Parallel reactions

Substance A decomposes simultaneously by two first-order unidirectional to products R and S:



At the beginning the reactor contained only pure substance A. 10 minutes after the initialization of the reaction the reaction mixture contained 56 mol. % A and 11 mol. % R. What is the composition of the reaction mixture (in molar per cents) after another 20 minutes?

[17.552 mol. % A; 20.612 mol. % R; 61.836 mol. % S; ($k_1 = 0.0145 \text{ min}^{-1}$, $k_2 = 0.0435 \text{ min}^{-1}$)]

Solution:

$$\tau_1 = 10 \text{ min}$$

$$c_A = c_{A0} - x_1 - x_2 \quad \frac{c_A}{\Sigma c} = 0.56 \quad c_A = 0.56 c_{A0}$$

$$c_R = x_1 \quad \frac{c_R}{\Sigma c} = 0.11 \quad c_R = 0.11 c_{A0}$$

$$c_S = x_2 \quad c_S = c_{A0} - c_A - c_R = c_{A0} - 0.56 c_{A0} - 0.11 c_{A0} = 0.33 c_{A0}$$
$$\Sigma c = c_{A0}$$

$$c_A = c_{A0} \cdot \exp [-(k_1 + k_2) \cdot \tau]$$

$$k_1 + k_2 = -\frac{1}{\tau_1} \cdot \ln \frac{c_A}{c_{A0}} = -\frac{1}{10} \cdot \ln 0.56 = 0.058 \text{ min}^{-1}$$

$$\frac{c_S}{c_R} = \frac{0.33 c_{A0}}{0.11 c_{A0}} = 3, \quad \frac{c_S}{c_R} = \frac{k_2}{k_1}, \quad k_2 = 3 k_1$$

$$k_1 + 3 k_1 = 0.058$$

$$k_1 = \frac{0.058}{4} = 0.0145 \text{ min}^{-1}$$

$$k_2 = 3 \cdot 0.0145 = 0.0435 \text{ min}^{-1}$$

$$\text{For } \tau_2 = \tau_1 + 20 = 30 \text{ min}$$

$$c_A = c_{A0} \cdot \exp [-0.058 \cdot 30] = 0.17552 c_{A0} \dots\dots\dots 17.552 \text{ mol.\% A}$$

$$c_S = 3 c_R$$

$$c_{A0} = c_A + c_R + c_S = 0.17552 c_{A0} + c_R + 3 c_R$$

$$\Rightarrow c_R = \frac{1-0.17552}{4} c_{A0} = 0.20612 c_{A0} \dots\dots\dots 20.612 \text{ mol.\% R}$$

$$c_S = 3 \cdot 0.20612 c_{A0} = 0.61836 c_{A0} \dots\dots\dots 61.836 \text{ mol.\% S}$$