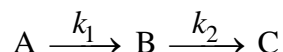


Problem 2-13 Consecutive reactions, composition of reaction mixture

Saponification of glycol diacetate occurs as the consecutive first-order reactions



at 18°C. For the rate constants the following values were found:

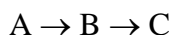
the saponification to the first degree $k_1 = 8.364 \cdot 10^{-7} \text{ s}^{-1}$,

the saponification to the second degree $k_2 = 2,574 \cdot 10^{-5} \text{ min}^{-1}$

What is the composition of reaction mixture (in mol. %) after 100 hours from the beginning of the reaction when the system contained only glycol diacetate.

[74 mol.% A, 24 mol.% B, 2 mol.% C]

Solution:



$$k_1 = 8.364 \cdot 10^{-7} \text{ s}^{-1}$$

$$k_2 = 2.574 \cdot 10^{-5} \text{ min}^{-1} = 2.574 \cdot 10^{-5} / 60 \text{ s}^{-1} = 4.29 \cdot 10^{-7} \text{ s}^{-1}$$

$$\tau = 100 \text{ h} = 3.6 \cdot 10^5 \text{ s}$$

$$c_{B0} = 0$$

Balance:

$$c_A = c_{A0} - x_1$$

$$c_B = c_{B0} + x_1 - x_2 = x_1 - x_2 \quad (c_{B0} = 0)$$

$$c_C = c_{C0} + x_2 = x_2 \quad (c_{C0} = 0)$$

$$\Sigma c = c_A + c_B + c_C = c_{A0}$$

$$c_A = c_{A0} \cdot \exp(-k_1 \cdot \tau) = c_{A0} \cdot \exp(-8.364 \cdot 10^{-7} \cdot 3.6 \cdot 10^5) = 0.74 c_{A0} \dots\dots\dots 74 \text{ mol. \% A}$$

$$c_B = c_{B0} \cdot e^{-k_2 \cdot \tau} + \frac{k_1 \cdot c_{A0}}{k_2 - k_1} \left[e^{-k_1 \cdot \tau} - e^{-k_2 \cdot \tau} \right]$$
$$= 0 + c_{A0} \cdot \frac{8.364 \cdot 10^{-7}}{4.29 \cdot 10^{-7} - 8.364 \cdot 10^{-7}} \cdot \left[\exp(-8.364 \cdot 10^{-7} \cdot 3.6 \cdot 10^5) - \exp(-4.29 \cdot 10^{-7} \cdot 3.6 \cdot 10^5) \right]$$

$$c_B = 0.24 c_{A0} \dots\dots\dots 24 \text{ mol. \% B}$$

$$\Sigma c = c_A + c_B + c_C = c_{A0}$$

$$0.74 c_{A0} + 0.24 c_{A0} + c_C = c_{A0}$$

$$c_C = c_{A0} - (0.74 c_{A0} + 0.24 c_{A0}) = 0.02 c_{A0} \dots\dots\dots 2 \text{ mol. \% C}$$