## Problem 2-06 Parallel reactions

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

$$(1) \qquad A \xrightarrow{k_1} R$$

$$(2) \qquad A \xrightarrow{k_2} S$$

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 min$^{-1}$, $k_2$ = 0.0435 min$^{-1}$)]

### Solution:

$\tau_1$ = 10 min

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

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

$c_S = x_2$ $\qquad c_S = c_{A0} - c_A - c_R = c_{A0} - 0.56\, c_{A0} - 0.11\, c_{A0} = 0.33\, c_{A0}$

$\Sigma c = c_{A0}$

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

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

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

$$k_1 + 3\, k_1 = 0.058$$

$$k_1 = \frac{0.058}{4} = 0{,}0145 \text{ min}^{-1}$$

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

For $\tau_2 = \tau_1 + 20 = 30$ min

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

$c_S = 3\, c_R$

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

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

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