Problem 2-10 Consecutive reactions, intermediate maximal concentration

The rate constants of the two first-order consecutive reactions

$$A \xrightarrow{k_1} B \xrightarrow{k_2} C$$

are $k_1 = 3.09{\cdot}10^{-4}\ \mathrm{s}^{-1}$ and $k_2 = 6.18{\cdot}10^{-3}\ \mathrm{min}^{-1}$. Calculate what time is needed to reach the maximal concentration of the intermediate B and the value of this concentration in case that the initial concentration of A was $c_{A0} = 0.2$ mol dm^{-3}.

[τ_{max} = 1.48 h , c_{Bmax} = 0.1155 mol dm^{-3}]

Solution:

$c_{A0} = 0.2$ mol dm^{-3}
$k_1 = 3.09{\cdot}10^{-4}\ \mathrm{s}^{-1}$ a
$k_2 = 6.18{\cdot}10^{-3}\ \mathrm{min}^{-1} = 6.18{\cdot}10^{-3}/60 = 1.03{\cdot}10^{-4}\ \mathrm{s}^{-1}$

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

maximum:

$$\frac{\mathrm{d}c_B}{\mathrm{d}\tau} = \frac{k_1 \cdot c_{A0}}{k_2 - k_1}\left[-k_1 \cdot e^{-k_1 \cdot \tau_{max}} + k_2 . e^{-k_2 \cdot \tau_{max}}\right] = 0$$

$$k_1 \cdot e^{-k_1 \cdot \tau_{max}} = k_2 . e^{-k_2 \cdot \tau_{max}}$$

$$\frac{k_1}{k_2} = e^{(k_1 - k_2) \cdot \tau_{max}}$$

$$\tau_{max} = \frac{\ln \frac{k_1}{k_2}}{k_1 - k_2} = \frac{\ln \frac{3.09 \cdot 10^{-4}}{1.03 \cdot 10^{-4}}}{3.09 \cdot 10^{-4} - 1.03 \cdot 10^{-4}} = 5333.07\ \mathrm{s} = 1.4814\ \mathrm{h}$$

$$c_{Bmax} = \frac{3.09 \cdot 10^{-4} \cdot 0.2}{1.03 \cdot 10^{-4} - 3.09 \cdot 10^{-4}} \cdot \left[\exp(-3.09 \cdot 10^{-4} \cdot 5333.07) - \exp(-1.03 \cdot 10^{-4} \cdot 5333.07)\right]$$

$$= 0.11547\ \mathrm{mol\ dm^{-3}}$$