$$x_A = x_{AEQ}\left(1 - e^{-\xi t}\right)$$

$$0.9682 = 0.9641\left(1 - e^{-5.288\times10^{-3}t}\right)$$

$$\frac{0.9682}{0.0941} = 1.0043 = 1 - e^{-5.288\times10^{-3}t}$$

$$= 0.0043 = -e^{-5.288\times10^{-3}t}$$

$$-0.0043 = e^{-5.288\times10^{-3}t}$$

ASIDE

$A \rightleftharpoons B$ ↳

glucose → Glucose 6P

⇅

Fructose 6P

↳ Fructose 1,6 P_2

What do you do to get all the * to react?

c)

$$\left.\begin{aligned} C_{Bo} &= 0 \\ \gamma &= 0 \\ \chi_{AEQ} &= 0.9834 \end{aligned}\right\}$$ SAME VALUES AS IN PART A)

$$C_A = C_{Ao}(1 - \chi_A)$$

$$C_{AEQ} = C_{Ao}(1 - \chi_{AEQ})$$

$$C_{AEQ} = 8.453\times10^{-7}(1 - 0.9834)$$

$$C_{AEQ} = 0.140\times10^{-7}\ mol/L$$

$$0.140\times10^{-7}\frac{mol}{L} \times \frac{182g}{mol} \times \frac{10^6\mu g}{g} = \underline{2.55ppb}$$

EXAMPLE 5

THE FOLLOWING REACTION IS SECOND ORDER IRREVERSIBLE:

$$A + 3B \rightarrow 2C$$

IF $C_{A0} = 100$ mmol/L & $C_{B0} = 250$ mmol/L

AT WHAT TIME WILL C_C REACH 80 mmol/L?

$k = 1.5 \times 10^{-4}$ L/mmol min

$$x_A = \frac{\gamma\left[e^{qt} - 1\right]}{\gamma e^{qt} - 1}$$

where $\gamma = \dfrac{C_{B0}}{3C_{A0}}$

$q = (C_{B0} - 3C_{A0})k$

$$r = \frac{C_{B0}}{3C_{A0}} = \frac{250}{3(100)} = 0.833$$

$$2 = (C_{B0} - 3C_{A0})k = (250 - 3(100))(1.5\times10^{-4})$$

$\frac{mmol}{L}$ L/mmol min

$$= -0.0075 \text{ min}^{-1}$$

$X_A = ?$ WHAT IS RELATIONSHIP BETWEEN A & C?

$$2\left(\text{\# moles of A consumed}\right) = \text{\# moles of C generated}$$

$$2(C_{A0} - C_A) = C_C - \cancel{C_{C0}}^{\,0}$$

$$2(C_{A0} - C_A) = C_C$$

$$2(100 - C_A) = 80 \rightarrow C_A = 60 \text{ mmol/L}$$

"AT WHAT TIME WILL C_C REACH 80 mmol/L?"

IS EQUIVALENT TO

"AT WHAT TIME WILL C_A REACH 60 mmol/L?"

$$X_A = \frac{C_{A0} - C_A}{C_{A0}} = \frac{100-60}{100} = 0.40$$

SO...

$$0.40 = \frac{0.833\left(e^{-0.0075t} - 1\right)}{0.833e^{-0.0075t} - 1}$$

$$\Downarrow$$

$$\underline{t = 19.1 \text{ min}}$$

WE COULD ALSO USE:

$$t = \frac{1}{2}\ln\left[\frac{\gamma - X_A}{\gamma(1-X_A)}\right]$$

6) MULTIPLE REACTIONS

a) INTRODUCTION

PARALLEL: REACTIONS WHICH USE SAME REACTANT(S)

$$A \rightarrow B$$
$$A \rightarrow C$$

SERIES: REACTIONS IN WHICH PRODUCT(S) OF ONE REACTION ARE REACTANT(S) FOR A SECOND REACTION

$$A \rightarrow B \rightarrow C$$

COMPLEX

$$\begin{tikzcd} A \arrow[r] \arrow[d] & B \arrow[r] \arrow[d] & D \\ C \arrow[r] & E & \end{tikzcd}$$

3 SERIES &

2 PARALLEL

EXAMPLE 6

$$\begin{tikzcd} A \arrow[r, "\#1"] \arrow[d, "\#2"'] & B \arrow[r, "\#3"] \arrow[d, "\#4"] & D \\ C \arrow[r, "\#5"'] & E & \end{tikzcd}$$

ALL FIRST ORDER RXNS!

GIVEN: k_1, k_2, k_3, k_4, k_5

$C_{A0}, C_{B0}, C_{C0}, C_{D0}, C_{E0}$

$$R_A = \frac{dc_A}{dt} = -k_1 c_A - k_2 c_A$$

$$R_B = \frac{dc_B}{dt} = +k_1 c_A - k_3 c_B - k_4 c_B$$

$$R_C = \frac{dc_C}{dt} = +k_2 c_A - k_5 c_C$$

$$R_D = \frac{dc_D}{dt} = +k_3 c_B$$

$$R_E = \frac{dc_E}{dt} = +k_5 c_C + k_4 c_B$$

USE SOFTWARE TO SOLVE MULTIPLE DIFF. EQN SIMULTANEOUSLY, OR WRITE YOUR OWN CODE!