b) ANALYSIS OF A SERIES REACTION

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

ALL FIRST ORDER

$$\frac{dC_A}{dt} = -k_1 C_A \qquad C_A = C_{A0} \text{ @ } t=0$$

$$\frac{dC_B}{dt} = k C_A - k_2 C_B \qquad C_B = C_{B0} \text{ @ } t=0$$

$$\boxed{C_A = C_{A0} e^{-k_1 t}}$$

$$\frac{dC_B}{dt} = k_1 C_{A0} e^{-k_1 t} - k_2 C_B$$

$$\underbrace{\frac{dC_B}{dt} + k_2 C_B}_{C_B} = \underbrace{k_1 C_{A0} e^{-k_1 t}}_{t}$$

THIS DIFFERENTIAL EQN IS SOLVED BY A PROCEDURE INVOLVING A HOMOGENEOUS SOLUTION & A PARTICULAR SOLUTION $C_B = C_B^H + C_B^P$

HOMOGENEOUS SOLN

$$\frac{dc_B^H}{dt} + k_2 c_B^H = 0$$

$$\boxed{c_B^H = A_0 e^{-k_2 t}}$$

DO NOT INSERT INITIAL CONDITION YET!

PARTICULAR SOLN

$$\frac{dc_B^P}{dt} + k_2 c_B^P = k_1 c_{A0} e^{-k_1 t}$$

TRY $c_B^P = A_1 e^{-k_1 t}$

$$\frac{dc_B^P}{dt} = -A_1 k_1 e^{-k_1 t}$$

$$-A_1 k_1 \cancel{e^{-k_1 t}} + k_2 A_1 \cancel{e^{-k_1 t}} = k_1 C_{A0} \cancel{e^{-k_1 t}}$$

$$-A_1 k_1 + k_2 A_1 = k_1 C_{A0}$$

$$A_1 (k_2 - k_1) = k_1 C_{A0}$$

$$A_1 = \frac{k_1 C_{A0}}{k_2 - k_1}$$

AS LONG AS $k_2 \neq k_1$

SO THE SOLUTION IS

$$C_B = C_B^H + C_B^P$$

$$C_B = A_0 e^{-k_2 t} + \frac{k_1 C_{A0}}{k_2 - k_1} e^{-k_1 t} \qquad k_1 \neq k_2$$

APPLY INITIAL CONDITION TO FIND A_0 $\quad C_B = C_{B0}$ @ $t = 0$

$$C_{B0} = A_0 (1) + \frac{k_1 C_{A0}}{k_2 - k_1} (1)$$

$$A_0 = C_{B0} - \frac{k_1 C_{A0}}{k_2 - k_1}$$

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

$$c_{B_{i+1}} = \left(k_1 c_{A_i} - (k_3 + k_4) c_{B_i}\right) \Delta t + c_{B_i}$$

PROGRAM....

$k_1 = 0.15\ min^{-1}$

$k_2 = 0.14\ min^{-1}$

$k_3 = 0.11\ min^{-1}$

$k_4 = 0.12\ min^{-1}$

$k_5 = 0.08\ min^{-1}$

$c_{A0} = 100\ mM$

$c_{B0} = 0$

$c_{C0} = 0$

$c_{D0} = 0$

$c_{E0} = 0$

$$\boxed{C_B = C_{B0} e^{-k_2 t} + \frac{k_1 C_{A0}}{k_2 - k_1}\left[e^{-k_1 t} - e^{-k_2 t}\right]} \quad k_1 \neq k_2$$

IF $C_{B0} = 0$

THEN $$C_B = \frac{k_1 C_{A0}}{k_2 - k_1}\left[e^{-k_1 t} - e^{-k_2 t}\right] \quad k_1 \neq k_2$$

IF $C_{B_0}=0$ FIND t_{MAX}, THE TIME AT WHICH B CONCENTRATION REACHES A MAXIMUM.

$$0 = \frac{dc_B}{dt} = \frac{k_1 C_{A0}}{k_2-k_1}\underbrace{\left[-k_1 e^{-k_1 t_{max}} + k_2 e^{-k_2 t_{max}}\right]}_{=0?}$$

$$k_1 e^{-k_1 t_{max}} = k_2 e^{-k_2 t_{MAX}}$$

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

$$\ln\left(\frac{k_1}{k_2}\right) = t_{max}(k_1 - k_2)$$

$$\boxed{t_{max} = \frac{\ln(k_1/k_2)}{k_1 - k_2}} \qquad k_1 \neq k_2$$

NOTE: BECAUSE OF STOICHIOMETRY

$$C_A + C_B + C_C = \text{CONSTANT} = C_{A0} + C_{B0} + C_{C0}$$

$$C_C = C_{A0} + C_{B0} + C_{C0} - C_B - C_A$$

EXAMPLE 7

let $C_{A0} = 100$

$C_{B0} = 0$

$C_{C0} = 0$

3 CASES

A) $k_1 = 0.025$ $k_2 = 0.10$ $k_2 > k_1$

B) $k_1 = 0.049$ $k_2 = 0.051$ $k_1 \cong k_2$

C) $k_1 = 0.10$ $k_2 = 0.025$ $k_1 > k_2$