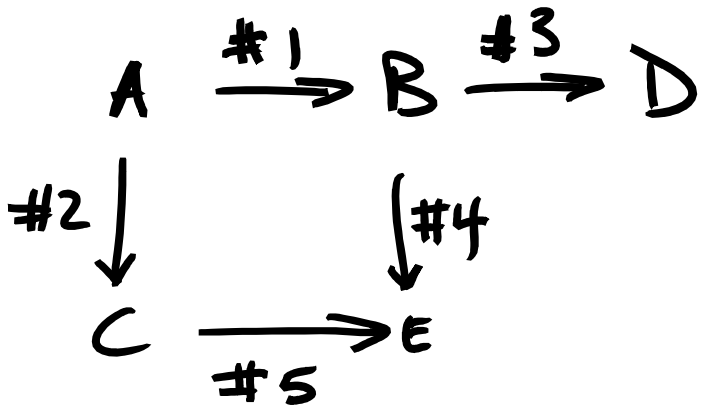
# EXAMPLE 6




ALL FIRST ORDER RXNS!

GIVEN: $k_1, k_2, k_3, k_4, k_5$

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

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

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

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

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

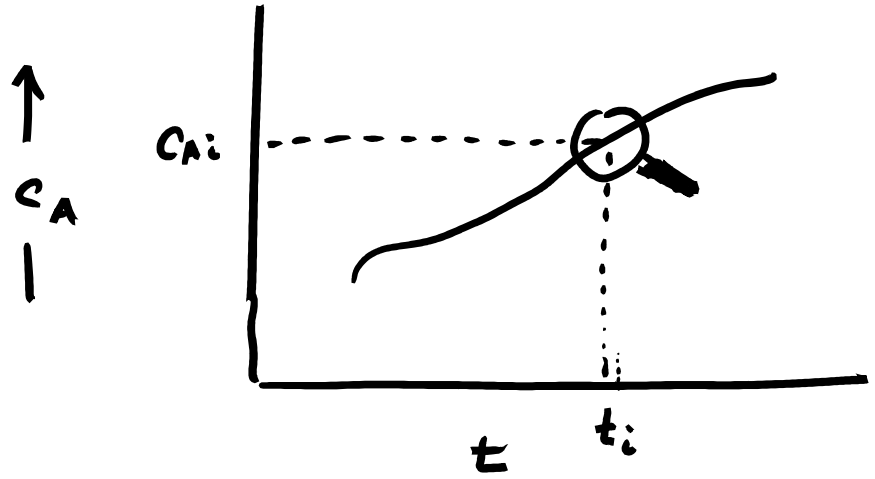
$$R_E = \frac{dc_E}{dt} = +k_5 c_C + k_4 c_B$$

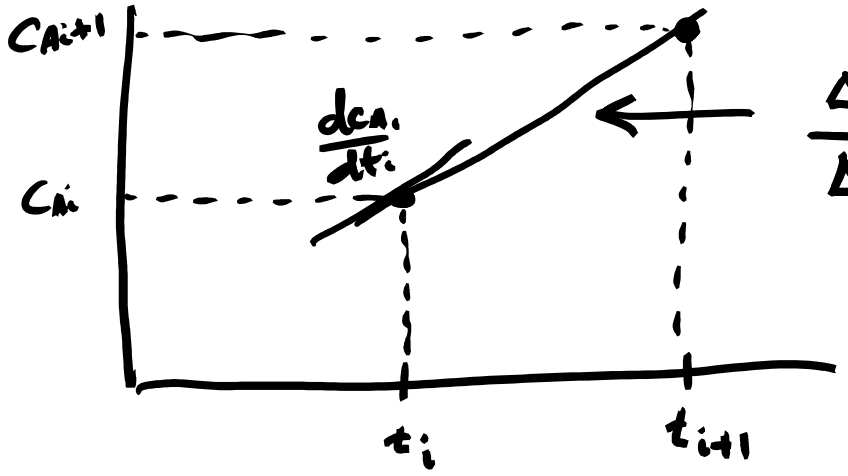
USE SOFTWARE TO SOLVE MULTIPLE DIFF. EQN SIMULTANEOUSLY, OR WRITE YOUR OWN CODE!

TO WRITE YOUR OWN CODE,

CHANGE DIFF EQNS INTO DIFFERENCE EQUATIONS

$$\frac{dc_A}{dt} \simeq \frac{\Delta c_A}{\Delta t} \qquad \frac{dc_B}{dt} \simeq \frac{\Delta c_B}{\Delta t} \quad \ldots \text{ etc.}$$




$$\frac{\Delta c_A}{\Delta t} = \frac{c_{A,i+1} - c_{A,i}}{t_{i+1} - t_i}$$

$$\lim_{\Delta t \to 0} \frac{\Delta c_A}{\Delta t} = \frac{dc_A}{dt}$$

$$* \quad \frac{dC_A}{dt} = -k_1 C_A - k_2 C_A = -(k_1 + k_2) C_A$$

$$\frac{C_A}{\Delta t} = \frac{C_{Ai+1} - C_{Ai}}{\Delta t} = -(k_1 + k_2) C_{Ai}$$

SOLVE FOR $C_{Ai+1}$

$$\boxed{C_{Ai+1} = -(k_1 + k_2) C_{Ai} \Delta t + C_{Ai}}$$

WE CAN CALCULATE THE NEXT VALUE FOR $C_A$ ($C_{Ai+1}$) GIVEN THE CURRENT VALUE ($C_{Ai}$)

AS LONG AS WE KNOW THE FIRST VALUE OF $C_A$ (INITIAL VALUE AT $t=0$, $C_{A0}$), THEN WE WILL BE ABLE TO "MARCH OFF IN TIME" ($\Delta t$ UNITS AT A TIME) TO PREDICT THE NEXT VALUE OF $C_A$. WE THEN USE THAT VALUE OF $C_A$ TO CALCULATE THE NEXT VALUE, AND SO FORTH...

$$C_{A1} = -(k_1 + k_2) C_{A0} \Delta t + C_{A0}$$

$$C_{A2} = -(k_1 + k_2) C_{A1} \Delta t + C_{A1}$$

$$C_{A3} = -(k_1 + k_2) C_{A2} \Delta t + C_{A2} \quad \ldots \text{ etc.}$$

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

$$c_{B\,i+1} = \left( k_1 c_{A\,i} - (k_3 + k_4) c_{B\,i} \right) \Delta t + c_{B\,i}$$

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PROGRAM ....

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

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

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

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

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

$c_{A0} = 100 \text{ mM}$

$c_{B0} = 0$

$c_{C0} = 0$

$c_{D0} = 0$

$c_{E0} = 0$