HOMEWORK DUE FRIDAY

WATCH DATES FOR NEXT TWO WEEKS

HELP|ZHELP SESSIONS

SARADA	ZHELP	1:00-2:00	SUN
SOMEWHERE IN DRIFTMIER	HELP	4:15-5:28	TUE
	HELP	6:50-8:00	THU

$$1 - x_A = e^{-kt}$$

$$\boxed{x_A = 1 - e^{-kt}}$$

WE CAN ALSO START WITH RESULT FROM FIRST-ORDER DERIVATION USING C_A.

$$C_A = C_{A0} e^{-kt}$$

$$\downarrow$$

$$C_{A0}(1 - x_A) = C_{A0} e^{-kt}$$

$$1 - x_A = e^{-kt}$$ ... SAME RESULT.

$$x_A = 1 - e^{-kt}$$

"kt" — DIMENSIONLESS "TIME CONSTANT"

NOTE: WHEN $t=0$ $e^{-kt}=1$ AND $x_A=0$

WHEN $t \to \infty$ $e^{-kt} \to 0$ AND $x_A \longrightarrow 1$

kt	x_A
0	0
1	0.632
2	0.865
3	0.950

"CONVERSION IS 95% WHEN TIME CONSTANT (kt) IS 3.0"

3) SECOND ORDER (BIMOLECULAR) IRREVERSIBLE SINGLE REACTION
STOICHIOMETRY = 1:1

$$A + B \rightarrow C$$

"SECOND ORDER" = RATE IS PROPORTIONAL TO CONCENTRATION TO THE SECOND POWER

"BIMOLECULAR" = THERE ARE TWO REACTANTS

$$R_A = \frac{dC_A}{dt} = -kC_A C_B$$

OVERALL ORDER IS TWO

AGAIN, CONC. OF "A" DECREASES WITH TIME

"SECOND ORDER RATE CONSTANT" = f(T)

UNITS ARE $\frac{\text{VOL}}{\text{MOLE} \cdot \text{TIME}}$

NOTE BECAUSE OF STOICHIOMETRY $R_A = R_B$
(EQUAL COEFFICIENTS)

GOAL: FIND C_A & C_B AS FUNCTIONS OF TIME

WE WILL SOLVE USING FRACTIONAL CONVERSIONS

$$X_A = \frac{C_{A0} - C_A}{C_A} \qquad C_A = C_{A0}(1 - X_A)$$

$$X_B = \frac{C_{B0} - C_B}{C_B} \qquad C_B = C_{B0}(1 - X_B)$$

$$\frac{d}{dt}\left[C_{A0}(1 - X_A)\right] = -k\, C_{A0}(1 - X_A)\, C_{B0}(1 - X_B)$$

$$\frac{d\chi_A}{dt} = k(1-\chi_A)\,C_{B0}(1-\chi_B)$$

NOTE EQN LOOKS LIKE

$$\frac{dx}{dt} = f(x,y)$$

WHAT IS RELATIONSHIP BETWEEN

χ_A & χ_B?

LOOK BACK AT CHEMICAL REACTION

$$A + B \rightarrow C$$

NUMBER OF MOLES OF "A" REACTED = NUMBER OF MOLES OF "B" REACTED

NUMBER OF MOLES OF "A" REACTED = NUMBER OF MOLES "A" AT BEGINNING − NUMBER OF MOLES OF "A" NOW

$$n_{A0} - n_A = n_{B0} - n_B$$

$$C_{A0} - C_A = C_{B0} - C_B \quad \text{(CONSTANT } V\text{)}$$

$$C_{A0} - C_{A0}(1 - X_A) = C_{B0} - C_{B0}(1 - X_B)$$

$$C_{A0}[1 - 1 + X_A] = C_{B0}[1 - 1 + X_B]$$

$$\boxed{C_{A0} X_A = C_{B0} X_B}$$

SUBSTITUTE INTO DIFF EQN.

$$\frac{d\chi_A}{dt} = k(1-\chi_A)(c_{B0} - c_{A0}\chi_A)$$

$$\frac{dx}{dt} = f(x)$$

let $\gamma = \frac{c_{B0}}{c_{A0}}$

$$\Downarrow$$

$$\frac{d\chi_A}{dt} = c_{A0} k (1-\chi_A)(\gamma - \chi_A)$$

IF $\gamma = 1$

$$\frac{dX_A}{dt} = C_{A0} k (1 - X_A)^2$$

$$\int_0^{X_A} \frac{dX_A}{(1-X_A)^2} = C_{A0} k \int_0^t dt = C_{A0} k t$$

$u = 1 - X_A$

$du = -dX_A$

$$-\int \frac{du}{u^2} = u^{-1} = (1-X_A)^{-1} \Big|_0^{X_A}$$

$$= \frac{1}{1-X_A} - 1 = C_{A0} k t$$