

Homework due Friday

Watch dates for next two weeks

HELP/ZHELP sessions

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

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

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

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

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

↓

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

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

... SAME RESULT.

$$\chi_A = 1 - e^{-kt}$$

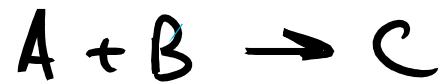
" kt " — DIMENSIONLESS "TIME CONSTANT"

NOTE: WHEN $t = 0$ $e^{-kt} = 1$ AND $\chi_A = 0$
 WHEN $t \rightarrow \infty$ $e^{-kt} \rightarrow 0$ AND $\chi_A \rightarrow 1$

$\frac{kt}{}$	$\frac{\chi_A}{}$
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



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

"BIMOLECULAR" = THERE ARE TWO REACTANTS

$$R_A = \frac{dC_A}{dt} = -k C_A C_B$$

AGAIN, CONC. OF "A"
DECREASES WITH TIME

← OVERALL ORDER IS TWO

"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

$$X_A = \frac{C_{A0} - C_A}{C_A}$$

$$X_B = \frac{C_{B0} - C_B}{C_B}$$

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

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

$$\frac{d}{dt} [C_{A0}(1 - X_A)] = -k \underbrace{C_{A0}(1 - X_A)}_{C_A} \underbrace{C_{B0}(1 - X_B)}_{C_B}$$

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

NOTE EQN
LOOKS LIKE

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

WHAT IS RELATIONSHIP BETWEEN
 $\chi_A \neq \chi_B$?

LOOK BACK AT CHEMICAL REACTION



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

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

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

$$C_{A0} - C_{A0}(1 - \chi_A) = C_{B0} - C_{B0}(1 - \chi_B)$$

$$C_{A0} [1 - 1 + \chi_A] = C_{B0} [1 - 1 + \chi_B]$$

$$C_{A0} \chi_A = C_{B0} \chi_B$$

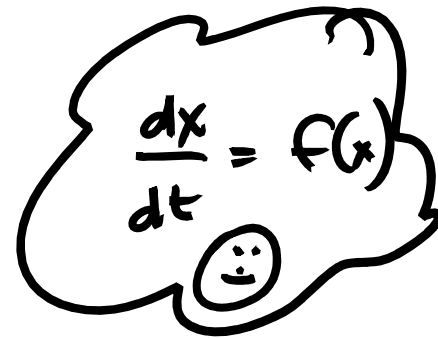
SUBSTITUTE INTO DIFF EQN.

$$\frac{dX_A}{dt} = k(1-X_A)(C_{B0} - C_{A0}X_A)$$

$$\text{let } \gamma = \frac{C_{B0}}{C_{A0}}$$



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



$$\text{IF } \gamma = 1 \quad \frac{d\chi_A}{dt} = c_{A0} k (1 - \chi_A)^2$$

$$\int_0^{\chi_A} \frac{d\chi_A}{(1 - \chi_A)^2} = c_{A0} k \int_0^t dt = c_{A0} k t$$

$$u = 1 - \chi_A$$

$$du = -d\chi_A$$

$$\begin{aligned} & \downarrow \\ & - \int \frac{du}{u^2} = u^{-1} = (1 - \chi_A)^{-1} \Big|_0^{\chi_A} \\ & = \frac{1}{1 - \chi_A} - 1 = c_{A0} k t \end{aligned}$$