Continuing on mass balance w/ chemical RXNs

from before

$$\frac{d(N_{C_2H_4Cl_2})}{dt} = -\frac{d(N_{C_2H_4})}{dt} = -\frac{d(N_{Cl_2})}{dt}$$

$$1 \qquad\qquad -1 \qquad\qquad -1$$

We can generalize these interrelationships between rates + apply to any chemical Reaction —

$$\alpha A + \beta B + \ldots \rightleftharpoons \rho R + \ldots$$

and $\alpha, \beta, \ldots$ are the <u>molar</u> stoichiometric coefficients.

$$\rho R + \ldots - \alpha A - \beta B - \ldots = 0$$

$$\boxed{\sum_i \nu_i I = 0}$$

ν_i : stoichoometric coefficient

I : species.

ν_i is positive for products
is negative for reactants

$$H_2O \rightleftharpoons H_2 + \frac{1}{2} O_2$$

$$\frac{1}{2} O_2 + H_2 - H_2O = 0$$

$\nu_{H_2} = +1$

$\nu_{O_2} = +\frac{1}{2}$

$\nu_{H_2O} = -1$

We need to Represent how far the chemical Reaction has gone.

N_i : number or quantity of species i in the system @ any time t
(@ = at)

Σ : sum $\quad \prod_i^n$ product.

$N_{i,0}$ is the amount at $t=0$

For a closed system N_i and $N_{i,0}$ through the variable $\boxed{X\text{: molar extent of Reaction}}$

$$\boxed{N_i = N_{i,0} + X \cdot \nu_i}$$

$$\boxed{X = \frac{N_i - N_{i,0}}{\nu_i}}$$

mathematical definition of molar extent of reaction.

electrolytic RXN -

$$H_2O \rightarrow \frac{1}{2} O_2 + H_2$$

initially 3.0 mol H_2O in a closed system. At some time later, 1.2 mol H_2

1.8 mol H_2O

a) Show that the molar extents of Reaction for H_2 and H_2O are equal.

b) Compute the number of moles of O_2 in the system.

i) Rewrite as $\boxed{\sum_i \nu_i I = 0}$

$$\boxed{H_2 + \frac{1}{2} O_2 - H_2O = 0}$$

$\nu_{H_2O} = -1$ $\nu_{H_2} = +1$ $\nu_{O_2} = +\frac{1}{2}$

From H_2

$$X = \frac{1.2 - 0}{1} = 1.2 \checkmark$$

H_2O:

$$X = \frac{1.8 - 3.0}{-1} = 1.2 \checkmark$$

b) $N_i = N_{i,0} + \nu_i X$

$= 0 + \frac{1}{2} \cdot 1.2$

$= 0.6$ mol

Good question —

Molar Extents of RXN have units

They tell you how far you're gone but not how fast you get there

we can relate this to speed of Reaction by $\frac{X}{t}$

Rate of change form of the mass balance w/ chemical Reaction: molar basis

$$\boxed{\frac{dN_i}{dt} = \sum_{k=1}^{K} (\dot{N}_i)_k + \nu_i \frac{dX}{dt}}$$

Accumulation In-n-Out Gen/Cons.

ethyl acetate and H_2O is formed by reaction between acetic acid and ethanol

$$\underset{A}{CH_3COOH} + \underset{E}{C_2H_5OH} \rightleftharpoons \underset{EA}{CH_3COOC_2H_5} + \underset{W}{H_2O}$$

The chemical Reaction for EA

☆ $$\frac{dC_{EA}}{dt} = \underline{K C_A \cdot C_E} - \underline{k' C_{EA} \cdot C_W}$$

$$K = 4.76 \cdot 10^{-4}\ m^3/kmol \cdot min$$

$$k' = 1.63 \cdot 10^{-4}\ m^3/kmol \cdot min$$

Reactor- Volume = $1\ m^3$

aqueous solution → 250 kg acetic acid
500 kg ethanol

density of solution is 1040 kg/m^3

Compute the number of moles of each component 100 minutes after reaction starts, and @ $t \to \infty$.

1) Identify initial mass + concentrations

2) determine N_A, N_E, N_W, N_{EA} in terms of X

3) Get differential equation for X
hint look @ ★

4) Solve said differential equation

1) C_A, C_E, C_W

$$C_A \rightarrow \frac{250\ kg/m^3}{60\ kg/kmol} \rightarrow 4.17\ kmol/m^3$$

$$C_E \rightarrow \frac{500\ kg/m^3}{46\ kg/kmol} \rightarrow 10.9\ kmol/m^3$$

$$C_W = \frac{1040 - 250 - 500}{18} \rightarrow 16.1\ kmol/m^3$$

→ make the $\boxed{\sum_i v_i I = 0}$

to get to b)