

Continuing on mass balance
w/ chemical RXNs

from before

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

\uparrow
 1

\uparrow
 -1

\uparrow
 -1

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



and α, β, \dots are the molar
stoichiometric coefficients.

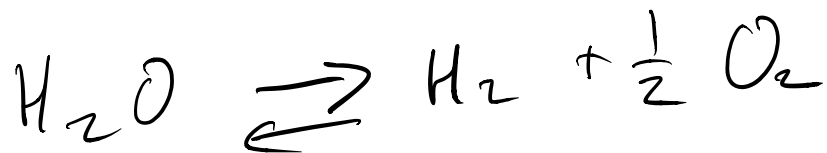
$$\gamma R + \dots - \alpha A - \beta B - \dots = 0$$

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

ν_i : stoichiometric
coefficient

I : species.

ν_i is positive for products
is negative for reactants



$$\nu_{\text{H}_2} = +1$$

$$\nu_{\text{O}_2} = +\frac{1}{2}$$

$$\nu_{\text{H}_2\text{O}} = -1$$

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
 Σ : sum \prod_i^n products \uparrow at

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

For a closed system N_i and $N_{i,0}$
through the variable

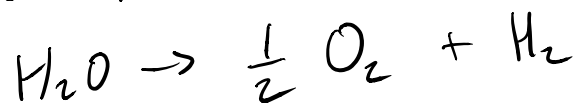
X : molar extent of
Reaction

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

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

mathematical definition of molar
extent of reaction.

electrolytic RXN -



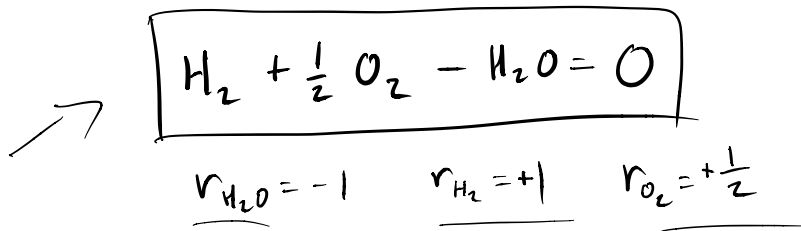
initially 3.0 mol H_2O in a closed system. At some time later, 1.2 mol H_2

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 $\sum_i \nu_i I = 0$



From H_2

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

$\text{H}_2\text{O}:$

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

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

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

$$= 0.6 \text{ mol}$$

Good question —

Molar Extents of RXN here units

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

we can relate this to speed of

Reaction by $\frac{X}{t}$

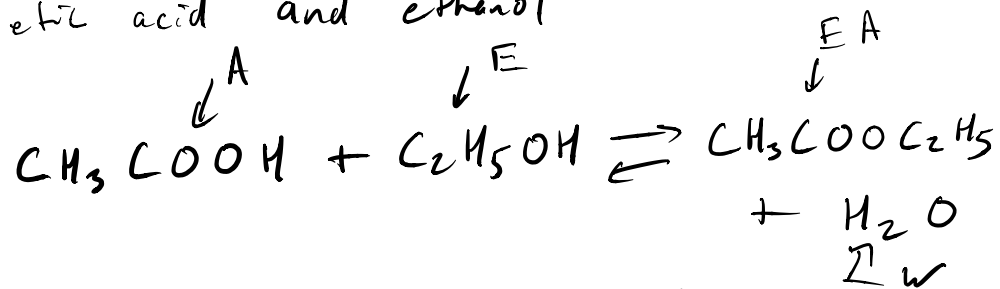
Rate of
change form
of the
mass balance
w/ chemical

Reaction: molar basis

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

\uparrow Accumulation \uparrow In-n-Out \uparrow Gen/Cons.

ethyl acetate ^{and H₂O} is formed by reaction between acetic acid and ethanol



The chemical Reaction for EA

$$\star \quad \frac{dC_{EA}}{dt} = \underbrace{K C_A \cdot C_E}_{\text{forward}} - \underbrace{K' C_{EA} \cdot C_w}_{\text{reverse}}$$

$$k = 4,76 \cdot 10^{-4} \text{ m}^3 / \text{kmol} \cdot \text{min}$$

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

Reactor- Volume = 1 m^3

aqueous solution \rightarrow 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 @ $t \rightarrow \infty$.

- 1) Identify initial mass + concentrations
- 2) determine N_A, N_E, N_W, N_{EA} in terms
 \rightarrow of X
- 3) Get differential equation for X
 hint look @ \star
- 4) Solve said differential equation

i) C_A, C_E, C_W

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

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

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

\rightarrow make the $\boxed{\sum_i v_i I = 0}$
 to get to b)