Tutorial 2

Q1

(a) $\underline{n}_1^T = [1, 2, 3, 0]$

$\underline{n}_2^T = [0.3, 1.65, 4.05, 0.7]$

(b) $[3, 5, 7, 2]$ & $[1, 4, 10, 3]$

Rxn: $3C + 3D - 2A - B = 0$

Principle: $\dfrac{n_j - n_{j0}}{\nu_j} = \epsilon$, indep. of species $\longrightarrow$ Stoichiometrically Compatible

Q2

Reactions:

$$\left.\begin{aligned} A_1 + A_2 - A_3 - A_4 &= 0 \\ -A_2 + 2A_3 - A_4 &= 0 \end{aligned}\right\} \Rightarrow \begin{aligned} m_1 + m_2 - m_3 - m_4 &= 0 \\ -m_2 + 2m_3 - m_4 &= 0 \end{aligned}$$

Prove $\frac{1}{2} m_4 < m_3 < 2m_4$

Step 1: Show that $m_3 + (>0) = m_4$

Step 2 Show that $\frac{1}{2} m_4 + (>0) = m_3$

Q3

You $\sum \nu_j A_j = 0$ $\quad \epsilon_1 = \frac{\Delta n_j}{\nu_j}$

Me $\sum \lambda \nu_j A_j = 0$ $\quad \epsilon_2 = \frac{\Delta n_j}{\lambda \nu_j}$

Q4

$$\overset{A_1}{Cu} + 2\overset{A_2}{H_2SO_4} = \overset{A_3}{CuSO_4} + 2\overset{A_4}{H_2O} + \overset{A_5}{SO_2}$$

At wts

$Cu = 63.5$

$S = 32$

$O = 16$

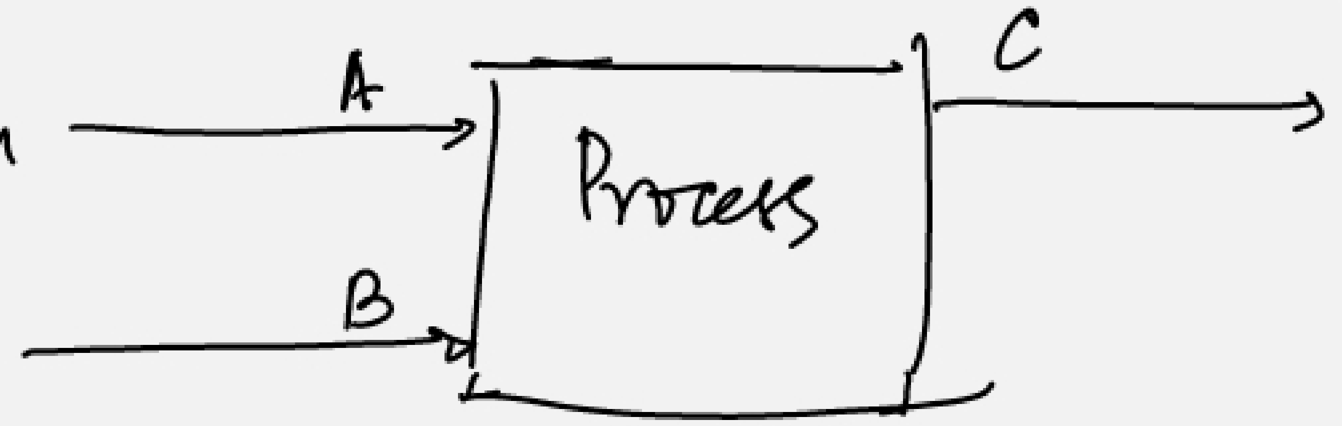
$H = 1$

PART 1

m_A Cu

kg	m_B
$m_{2B} =$	
$m_{4B} =$	

H_2SO_4 acid



m_C

$CuSO_4$ m_{3C}

H_2O m_{4C}

$SO_2 = m_{5C} = 1$ kg

II Part H_2SO_4

~~H_2O~~

Part 2: $Cu = 1000$ gm $= m_A$

$H_2SO_4 = 0.94 \times 15000 = m_{2B}$ ← Compare with H_2SO_4 needed $= \frac{2 \times 98}{63.55} \times 1000$

Cal excess H_2SO_4; Cal H_2O = Water from 94% acid + Water produced

Back to Stoichiometry

Single Rxn $\sum_{j=1}^{S} \nu_j A_j = 0 \longrightarrow \underline{\nu}^T \underline{a} = 0$

$$\Downarrow$$

$$\underline{\nu}^T \underline{m} = 0$$

$$\underline{\nu} = \begin{bmatrix} \nu_1 \\ \nu_2 \\ \vdots \\ \nu_S \end{bmatrix} \qquad \underline{a} = \begin{bmatrix} A_1 \\ A_2 \\ \vdots \\ A_S \end{bmatrix}$$

Multiple Rxn Systems: 'R' reactions

S.C. of A_j in Rxn i = ν_{ij} $\longrightarrow$ i^{th} reaction $\sum \nu_{ij} A_j = 0$; $i = 1(1)R$

$\overset{A_1}{NH_3} + \overset{A_2}{EtO} \longrightarrow \overset{A_3}{MEA}$

$MEA + EtO \longrightarrow \overset{A_4}{DEA}$

$DEA + EtO \longrightarrow \overset{A_5}{TEA}$

$-A_1 - A_2 + A_3 = 0$

$-A_2 - A_3 + A_4 = 0$

$-A_2 - A_4 + A_5 = 0$

$$\begin{array}{ccccc} A_1 & A_2 & & & \end{array}$$

$$\begin{bmatrix} -1 & -1 & 1 & 0 & 0 \\ 0 & -1 & -1 & 1 & 0 \\ 0 & -1 & 0 & -1 & 1 \end{bmatrix} \begin{bmatrix} A_1 \\ A_2 \\ A_3 \\ A_4 \\ A_5 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}$$

Each row $\underline{\underline{N}} \rightarrow$ Rxn

Each col $\rightarrow$ Species

$$\boxed{\underline{\underline{N}}\, \underline{a} = \underline{0}}$$

$$\underline{\underline{N}} = \begin{bmatrix} \nu_{11} & \nu_{12} & \cdots & \nu_{1j} & \cdots & \nu_{1s} \\ \nu_{21} & \nu_{22} & & \vdots & & \vdots \\ \vdots & \vdots & & \nu_{ij} & & \vdots \\ \nu_{R1} & \nu_{R2} & & \nu_{Rj} & \cdots & \nu_{Rs} \end{bmatrix} = \{\nu_{ij}\}_{R \times s}$$

$$\underset{R\times S}{\underline{\underline{N}}}\ \underset{S\times 1}{\underline{a}} = \underset{R\times 1}{\underline{0}}$$

$$\downarrow$$

$\underline{\underline{N}}\,\underline{m} = \underline{0}$ → mass balances for individual Rxns

$R \leq s$

If Rank of $\underline{\underline{N}} = R$ → Rxns are l. i

Ex: for NH_3-EtO-MEA-DEA-TEA system

$$\underline{m} = \begin{bmatrix} 17 \\ 44 \\ 61 \\ 105 \\ 149 \end{bmatrix}$$

$$\underline{\underline{N}}\,\underline{m} \overset{?}{=} 0$$

Extent of reaction no i $= \epsilon_i = \dfrac{\text{Change in moles of } A_j \text{ due to rxn } i}{\nu_{ij}} = \dfrac{(\Delta n_j)_{\text{Rxn } i}}{\nu_{ij}}$

$$\boxed{\Delta n_j = \underbrace{n_j - n_{j0}} = \sum_{i=1}^{R} \nu_{ij}\epsilon_i} \quad j = 1(1)S$$

In this set of S equations, only R are independent $\Rightarrow$ Only R of the S Columns are independent

$$\underline{\epsilon} = \begin{bmatrix} \epsilon_1 \\ \epsilon_2 \\ \vdots \\ \epsilon_R \end{bmatrix}$$ gives info on <u>RXNS</u>

$$\boxed{\underline{n} - \underline{n}_0 = \underline{\underline{N}}^T \underline{\epsilon}}$$

$S \times 1 \quad S \times 1 \quad S \times R \quad R \times 1$

How do we 'follow' a MRS ?

! Find 'R' L.i Columns (Species) $\rightarrow$ follow changes in their mole numbers

$$n_j - n_{j0} = \sum \nu_{ij} \epsilon_i \qquad j = 1(1)\underline{\underline{R}}$$

Solve this to get $\epsilon_1 \cdots \epsilon_R$ at diff times

$$n_k - n_{k0} = \sum \nu_{ik} \epsilon_i \qquad k = R, R+1, \cdots S$$

System degrees of freedom $= R$