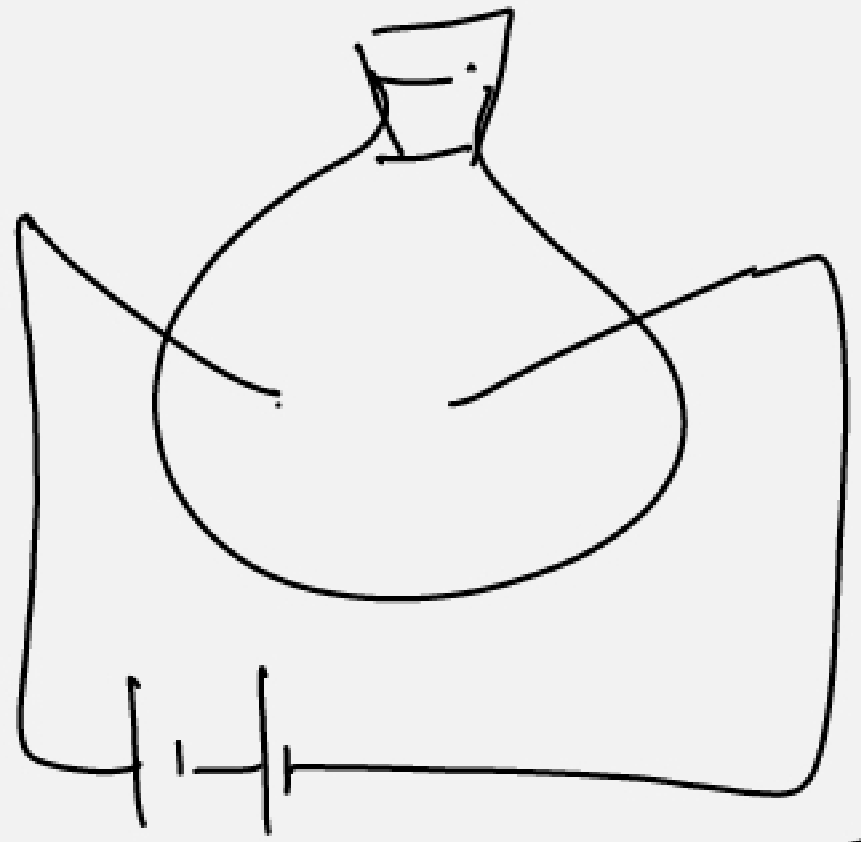
$$\sum_{j=1}^{S} \nu_j A_j = 0$$

A_j product $\Rightarrow \nu_j > 0$

A_j reactant $\Rightarrow \nu_j < 0$

$\nu \Rightarrow$ 'nu'

$$\left.\begin{aligned} 2H_2 + O_2 &= 2H_2O \\ H_2 + \tfrac{1}{2}O_2 &= H_2O \end{aligned}\right\}$$



<u>Performance</u>: How much of product?
Which product?
How much time?

$\boxed{\text{Nature}}$ $\left\{\begin{array}{l} \underline{\text{Stoichiometry}} \\ \text{Thermodynamics} \\ \text{Kinetics} \end{array}\right.$

Nurture $\left\{\begin{array}{l} \text{Reactor} \\ \text{Conditions} \\ \text{Presence of Catalyst} \\ \ldots\ldots \end{array}\right.$

__Stoichiometry__ :

$$\sum_{j=1}^{S} \nu_j A_j = 0$$

Change in moles of $A_j \propto \nu_j$

$$\frac{n_j - n_{j0}}{\nu_j} = \frac{\Delta n_j}{\nu_j} = \epsilon \quad \text{independent of species}$$

> 0

$$n_j = n_{j0} + \nu_j \epsilon$$

$\epsilon \rightarrow$ measure of 'how much' reaction has occurred $[=]$ moles $\Leftarrow$ Closed System $\boxed{n_{j0} \downarrow n_j}$

Open systems in St. State $\xrightarrow[\text{Reactants}]{} \boxed{} \xrightarrow[\text{Products}]{}$ $\Rightarrow$ $\dfrac{\Delta F_j}{\nu_j} = \text{Const } \epsilon$ moles/sec

mol/s

1) Units
2) magnitude depends on the stoich. eq.

ε = Reaction extent

Another measure of 'amount of Rxn': Conversion → Reactant
X

$$\frac{n_{j0} - n_j}{n_{j0}} = X_j = \text{Conversion of } A_j$$

$$2H_2 + O_2 = 2H_2O$$

	H_2	O_2	H_2O
Time 0	200 mol	200 mol	0
Time t	100 mol	150 mol	100
X	50%	25%	—

$$\varepsilon = \frac{-100}{-2} = 50$$

$$X_{H_2} = \frac{200 - 100}{200} = 50\%$$

$$X_{O_2} = \frac{200 - 150}{200} = 25\%$$

Comparison

Conversion	Reaction Extent
$0 \leq X_j \leq 1$	Can be anything
Dimensionless	moles (or mol/s)
Species (Reactt) dependent	Reaction dependent
Independent of Stoich descripn.	Dependent on Stoichio descripn.
Not suitable for multiple Rxns	Suitable for M.R

What does Stoichiometry do for us:

1) $\dfrac{\Delta n_j}{\nu_j} = \xi \rightarrow$ Progress of (a single) rxn requires only one species to be measured

2) ✓ Limiting Reactt

$$2H_2 + O_2 = 2H_2O$$

200 mol 200 mol

$$\min_{\text{for all reactts}} \frac{n_{j0}}{|\nu_j|}$$

H_2: $\dfrac{200}{2} = 100$

O_2: $\dfrac{200}{1} = 200$

$X \rightarrow$ always referred to L.R

$$\sum \nu_j A_j = 0 \leftarrow A_j \text{ is LR}$$

Conversion $X = \dfrac{n_{10} - n_1}{n_{10}}$

Extent $= \dfrac{n_j - n_{j0}}{\nu_j} = \dfrac{n_1 - n_{10}}{\nu_1} = \dfrac{-n_{10}X}{\nu_1}$

$$\varepsilon = \frac{n_{10}\,X}{(-\nu_1)}$$

Calculation of Comp Changes

$$n_j = n_{j0} + \nu_j \varepsilon$$

ε [=] moles

$$n_j = n_{j0} + \frac{\nu_j}{-\nu_1} n_{10} X$$

$$2H_2 + O_2 = 2H_2O$$

(R) Multiple Reactions: (Reaction networks)

$$\sum_{j=1}^{S} \nu_{ij} A_j = 0 \longrightarrow i^{th} \text{ reaction}$$

$$i = 1(1)R$$

$$\left.\begin{aligned} 2H_2 + O_2 &= 2H_2O \\ H_2 + O_2 &= H_2O_2 \end{aligned}\right\}$$

Single Rxn $\quad \nu_1 A_1 + \nu_2 A_2 + \cdots + \nu_S A_S = 0$

$$\begin{bmatrix} \nu_1 & \nu_2 & \cdots & \nu_S \end{bmatrix} \begin{bmatrix} A_1 \\ A_2 \\ \vdots \\ A_S \end{bmatrix} = 0$$

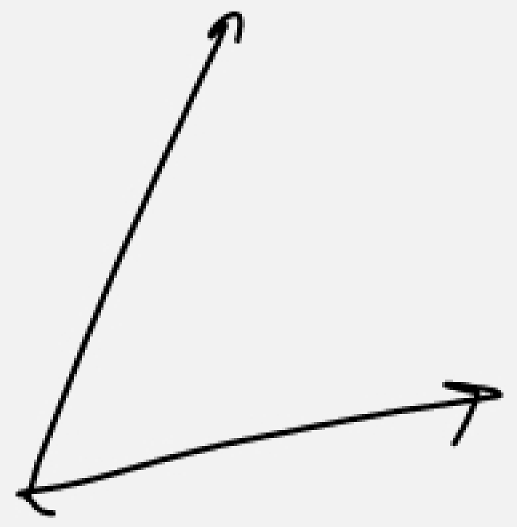
Vectors & matrices:

$\vec{a} = (a_1 \;\; a_2 \;\; a_3)$

$\vec{a} = a_1 \hat{i} + a_2 \hat{j} + a_3 \hat{k}$

$\vec{b} = b_1 \hat{i} + b_2 \hat{j} + b_3 \hat{k}$

$\bar{a} + \bar{b} = (a_1 + b_1)\hat{i} + (a_2 + b_2)\hat{j} + (a_3 + b_3)\hat{k}$



$\lambda \vec{a} = \lambda a_1 \hat{i} + \lambda a_2 \hat{j} + \lambda a_3 \hat{k}$

Dot: $\vec{a} \cdot \vec{b} = a_1 b_1 + a_2 b_2 + a_3 b_3$

Stoich vector

$\vec{\nu} = [\nu_1 \;\; \nu_2 \;\; \nu_3 \cdots \nu_S]$

Species vector

$\vec{a} = [A_1 \;\; A_2 \cdots\cdots A_S]$

$\sum \nu_j A_j = 0 \qquad \nu_1 A_1 + \nu_2 A_2 + \cdots\cdots + \nu_S A_S = 0$

$$\vec{v} = \begin{bmatrix} v_1 \\ v_3 \\ \vdots \\ v_5 \end{bmatrix} \qquad \vec{a} = \begin{bmatrix} A_1 \\ A_2 \\ \vdots \\ A_8 \end{bmatrix}$$

$$\vec{v}^T = \begin{bmatrix} v_1 & v_2 & \cdots & v_5 \end{bmatrix}$$

Square

$$\bar{\bar{A}} = \begin{bmatrix} a & b & c \\ p & q & r \\ x & y & z \end{bmatrix} \qquad \bar{\bar{A}}^T = \begin{bmatrix} a & p & x \\ b & q & y \\ c & r & z \end{bmatrix}$$

$$\begin{bmatrix} a & b & c & d \\ p & q & r & s \\ x & y & z & t \end{bmatrix} \begin{bmatrix} 1 & 3 \\ 2 & 2 \\ 3 & 5 \\ 4 & 6 \end{bmatrix} = \begin{bmatrix} a+2b+3c+4d & 3a+2b+5c+6b \\ p+2q+3r+4s & \\ & \end{bmatrix}$$

$3 \times 4 \qquad 4 \times \underline{2} \qquad 3 \times 2$

$$\underline{v}^T \underline{A} = \underbrace{\begin{bmatrix} v_1 & v_2 & \cdots & v_s \end{bmatrix}}_{1 \times s} \underbrace{\begin{bmatrix} A_1 \\ A_2 \\ \vdots \\ A_s \end{bmatrix}}_{s \times 1} \Rightarrow v_1 A_1 + v_2 A_2 + \cdots + v_s A_s = 0$$

$$\sum v_j A_j = 0$$