STOICHIOMETRY FUNDAMENTALS

Three types of stoichiometric relations. Each has set of stoichiometric coefficients which relate consumption/formation of a compound to other reactants and products in a particular reaction:

Molar:

$$\mathbf{a_1A_1 + a_2A_2 + \ldots + a_kA_k \rightarrow a_{k+1}A_{k+1} + a_{k+2}A_{k+2} + \ldots + a_mA_m}$$

where A_i are reactants for i = 1 → k and products for i = k+1 → m

And a_i are stoichiometric coefficients

Characteristics of molar stoichiometric relations:

Example:

$$\mathbf{1C_6H_{12}O_6 + 6O_2 \rightarrow 6CO_2 + 6H_2O}$$

Units: moles, molecules
Element mass is conserved
Charge is conserved

Typically, stoichiometric coefficients are normalized to a reference reactant or product, which then has a stoichiometric coefficient of "1."

Mass:

$$\mathbf{1A_1 + \Psi_2A_2 + \ldots + \Psi_{k+1}A_{k+1} \rightarrow \Psi_{k+2}A_{k+2} + \ + \Psi_mA_m}$$

Where Ψ_i are stoichiometric coefficients

And $\Psi_i = \dfrac{a_i(\text{MW of } A_i)}{a_1(\text{MW of } A_1)}$ for i = 2 → m

Note that mass stoichiometric coefficients are normalized by the molecular weight of the reference compound (typically reactant 1).

Units: mass (grams, kilograms)
Charge and element mass is not conserved

Total mass of reactants = total mass of products

That is:

$$\sum_{i=1}^{k} \Psi_i = \sum_{i=k+1}^{m} \Psi_i$$

Example:

$$\mathbf{C_6H_{12}O_6 + 1.067O_2 \rightarrow 1.467CO_2 + 0.6H_2O}$$

Reference compound is glucose, MW = 180

$\Psi_1 = 1$

$\Psi_2 = 6(32)/180 = 1.067$ g-O_2/g-glucose

$\Psi_3 = 6(44)/180 = 1.467$ g-CO_2/g-glucose

$\Psi_4 = 6(18)/180 = 0.60$ g-H_2O/g-glucose

balance: 1 + 1.067 = 2.067
1.467 + 0.6 = 2.067

COD (electron):

$$\mathbf{1A_1 + Y_2A_2 + \ldots + Y_{k+1}A_{k+1} \rightarrow Y_{k+2}A_{k+2} + \ + Y_mA_m}$$

where the reference compound is COD and the stoichiometric coefficients, Y_i are in units of mass COD

$Y_1 = 1$

$$Y_i = \frac{a_i(MW - A_i)(COD_i)}{a_1(MW - A_1)(COD_1)} = \Psi_i \frac{COD_i}{COD_1}$$

Where COD_i is the COD equivalent of the ith compound. For example the COD equivalent of glucose is 6*32/180 = 1.067 g-COD/g-glucose (see molar stoichiometry above).

Other useful COD equivalents: COD_{cells} ($C_5H_7NO_2$) = 5(32)/113 = 1.42 g-COD/g-cells

$$COD_{O2} = -1 \text{ g-COD/g-}O_2$$

COD equivalent of water, CO_2, and any other compound not involved in exchange of electrons is zero.

Units: g-COD
COD mass is conserved

Example:

$$\mathbf{1C_6H_{12}O_6–COD + (-1)O_2 \rightarrow 0CO_2 + 0H_2O}$$

Balance: 1 – 1 = 0
0 + 0 = 0