ATOMIC NUMBER DENSITY

Number of Atoms (n) and Number Density (N)

The number of atoms or molecules (n) in a mass (m) of a pure material having atomic or molecular weight (M) is easily computed from the following equation using Avogadro's number ($N_A = 6.022\times10^{23}$ atoms or molecules per gram-mole):

$$n = \frac{m\,N_A}{M} \tag{1}$$

In some situations, the *atomic number density* (N), which is the concentration of atoms or molecules per unit volume (V), is an easier quantity to find when the material density (ρ) is given

$$N = \frac{n}{V} = \frac{\rho\,N_A}{M} \tag{2}$$

Number Density for Compounds

For a chemical compound (mixture) Z, which is composed of elements X and Y, the number (atom) density of the compound is calculated from

$$N_Z = N_{mix} = \frac{\rho_{mix}\,N_A}{M_{mix}} \tag{3}$$

In some cases, the desired quantity is the number density of the compound constituents. Specifically, if $Z = X_p\,Y_q$, then there are p atoms of X and q atoms of Y for every molecule of Z; hence

$$N_X = p\,N_Z \qquad N_Y = q\,N_Z \tag{4}$$

Example: Calculate the number density of natural uranium in UO_2 with $\rho_{UO_2} = 10.5\ \text{g/cm}^3$.

$$N_U = N_{UO_2} = \frac{\rho_{UO_2}\,N_A}{M_{UO_2}} = \frac{(10.5\ \text{g/cm}^3)(6.022\times10^{23}\ \text{atoms/mol})}{[238.0289 + 2(15.9994)]\ \text{g/mol}} = 2.34\times10^{22}\ \text{atoms/cm}^3$$

Number Density Given Atom Fraction (Abundance)

Oftentimes, it is necessary to compute the concentration of an individual isotope j given its fractional presence (abundance) γ_j in the element

$$\gamma_j = \frac{\text{Number of atoms of isotope } j}{\text{Total number of atoms of the element}} \tag{5}$$

Many times, the fraction γ_j is stated as an atom percent, which is abbreviated a/o. The atomic number density of isotope j is then

$$N_j = \gamma_j\,N_{elem} = \frac{\gamma_j\,\rho_{elem}\,N_A}{M_{elem}} \tag{6}$$

If the element has a non-natural abundance of its isotopes (that is, the elemental material is either *enriched* or *depleted*), then it is necessary to compute the atomic weight of the element (M_{elem}) from the sum of all the atomic masses of the isotopes (M_j) rather than use the tabulated M_{elem} value found in a reference

$$M_{elem} = \sum \gamma_j\,M_j \tag{7}$$

Example: Find the U-235 concentration for 3 a/o in UO_2.
Solution: To solve this example, Equations (4), (3) and (7) are progressively substituted into Eq. (6).

$$\begin{aligned} N_{\text{U-235}} &= \gamma_{\text{U-235}}\, N_{\text{U}} = \gamma_{\text{U-235}}\, N_{\text{UO}_2} \\ &= \gamma_{\text{U-235}} \frac{\rho_{\text{UO}_2}\, N_{\text{A}}}{M_{\text{UO}_2}} = \frac{\gamma_{\text{U-235}}\, \rho_{\text{UO}_2}\, N_{\text{A}}}{\gamma_{238}\, M_{238} + \gamma_{235}\, M_{235} + 2\, M_{\text{O}}} \\ &= \left(0.03 \frac{\text{atoms-}^{235}\text{U}}{\text{atoms - U}} \right) \frac{(10.5\,\text{g/cm}^3)(6.022\times10^{23}\ \text{atoms/mol})}{[(238.05)(0.97)+(235.04)(0.03)+2(15.9994)]\,\text{g/mol}} \\ &= 7.03\times10^{20}\ \text{atoms/cm}^3 \end{aligned}$$

<u>Number Density Given Weight Fraction (Enrichment)</u>

Other times, when working with nuclear fuels such as uranium, the *enrichment* may be specified in terms of weight percent or weight fraction, ω_i, of isotope i:

$$\omega_i = \frac{Mass\ of\ isotope\ i}{Total\ mass\ of\ the\ element} \tag{8}$$

The atomic number density of isotope i is

$$N_i = \frac{\rho_i\, N_{\text{A}}}{M_i} = \frac{\omega_i\, \rho_{elem}\, N_{\text{A}}}{M_i} \tag{9}$$

Clearly, if the material is enriched, then the atomic weight of the material differs from its natural reference value, and the enriched atomic weight, if needed, should be computed from

$$\frac{1}{M_{elem}} = \sum_i \frac{\omega_i}{M_i} \tag{10}$$

Example: Find the U-235 concentration for 4% enriched UO_2.
Solution: First, compute the molecular weight of the enriched uranium, which is essentially 4% U-235 and 96% U-238 since the U-234 component is negligible.

$$\frac{1}{M_{\text{U}}} = \frac{\omega_{\text{U-235}}}{M_{\text{U-235}}} + \frac{\omega_{\text{U-238}}}{M_{\text{U-238}}} = \frac{0.04}{235.04} + \frac{0.96}{238.05}$$

$$M_{\text{U}} = 237.9\ \text{g/mol}$$

Next, use Equation (9) and the fact that $\rho_{\text{U}} = \rho_{\text{UO}_2} \frac{M_{\text{U}}}{M_{\text{UO}_2}}$

$$\begin{aligned} N_{\text{U-235}} &= \frac{\omega_{\text{U-235}}\, \rho_{\text{U}}\, N_{\text{A}}}{M_{\text{U-235}}} = \frac{\omega_{\text{U-235}}\, N_{\text{A}}}{M_{\text{U-235}}} \rho_{\text{UO}_2} \frac{M_{\text{U}}}{M_{\text{UO}_2}} \\ &= \left(0.04 \frac{\text{g-}^{235}\text{U}}{\text{g - U}} \right) \frac{(6.022\times10^{23}\ \text{atoms/mol})(10.5\,\text{g - UO}_2/\text{cm}^3)}{235.04\,\text{g-}^{235}\text{U/mol}} \left(\frac{237.9\,\text{g - U}}{[237.9+2(16.00)]\text{g - UO}_2} \right) \\ &= 9.49\times10^{20}\,\text{atoms/cm}^3 \end{aligned}$$