University of Pittsburgh

ME/ENGR 2100 Fundamentals of Nuclear Engineering

Radiation and Nuclear Reactions:

Calculating Atom Density

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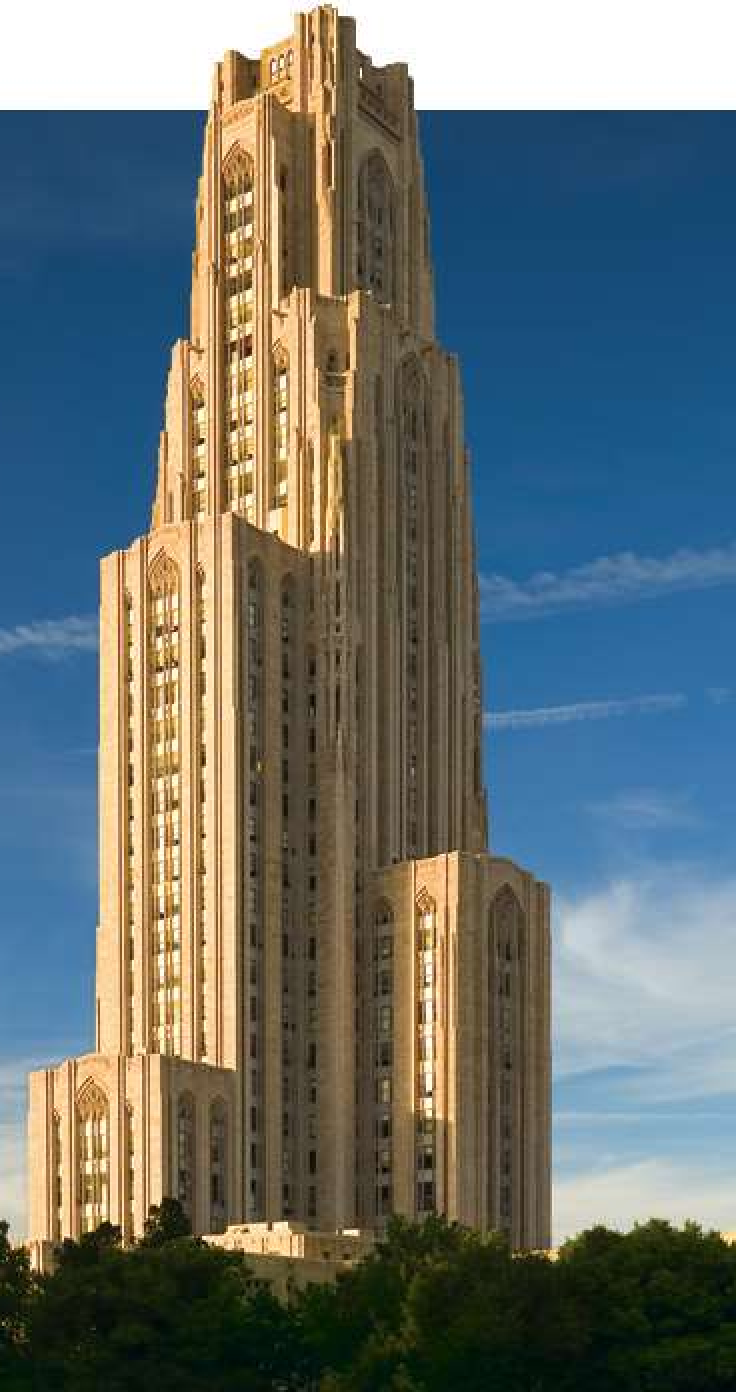

Relevant Reading Assignments

- Chapter 2/3 of "Introduction to Nuclear Engineering," Lamarsh and Baratta, 3rd edition, Prentice-Hall (2001)
- Chapter 2 of "Nuclear Engineering: Theory and Technology of Commercial Nuclear Power," Knief, 2nd edition, American Nuclear Society (1992, reprint by ANS 2008)
- Chapter 2 of "Nuclear Reactor Analysis," Duderstadt and Hamilton, Van Nostrand (1976)
- Module 1 of DOE Fundamentals Handbook, "Nuclear Physics and Reactor Theory," U.S.DOE (1993)Available at:

https://www.standards.doe.gov/standards-documents/1000/1019-bhdbk-1993-v1

- Not required but useful and clear is the discussion of nuclear masses and binding energies at the beginning of Chapter 7 of "Concepts of Nuclear Physics" by Bernard L. Cohen, McGraw-Hill, 1971, available in most scientific libraries.

Learning Objectives

- Calculate the atomic density of different types of materials

Calculating Number Density

- Calculating macroscopic cross sections requires calculation of the number density of nuclei in a material.
  - This information can be calculated using Avogadro's number.

Avogadro's Number $N_A = 6.022 \times 10^{23}$ atoms/mol

Atomic mass of atom in amu = Mass [g] per mol of atoms

$$N = \rho N_A / A$$

N = Atomic number density
ρ = Material density
N_A = Avogadro's Number
A = Atomic mass

Units: [atoms/cm^3] = [g/cm^3] × [atoms/mol] / [g/mol]

Number density of an element

- The density of sodium is 0.97 g/cm^3. Calculate its atom density.
  - The atomic weight of sodium is 22.990.

$$N = \frac{0.97 \frac{\text{g}}{\text{cm}^3} * 0.6022x10^{24} \frac{\text{atoms}}{\text{mol}}}{22.990 \frac{\text{g}}{\text{mol}}} = 0.0254x10^{24} \frac{\text{atoms}}{\text{cm}^3}$$

- To find number density of individual Na isotopes we would multiply by abundance

Number density of molecules

- Can also use this equation to find number density of molecules, and atoms within a molecule
- The density of water is 1.0 g/cm^3. Compute the molecular density of water, the atom densities of hydrogen and oxygen, and the atom density of deuterium (relative abundance 0.015 a/o).
  - The atomic weights of H and O are 1.00797 and 15.994, so the molecular weight of water is 2 * 1.00797 + 15.994 = 18.0153.

$$N_{wat} = \frac{1.0\frac{\text{g}}{\text{cm}^3} * 0.6022x10^{24}\frac{\text{molecules}}{\text{mol}}}{18.0153\frac{\text{g}}{\text{mol}}} = 0.03343x10^{24}\frac{\text{molecules}}{\text{cm}^3}$$

$$N_H = 2 * 0.03343x10^{24}\frac{\text{atoms}}{\text{cm}^3} = 0.6686x10^{24}\frac{\text{atoms}}{\text{cm}^3}$$

$$N_O = 1 * 0.03343x10^{24}\frac{\text{atoms}}{\text{cm}^3} = 0.03343x10^{24}\frac{\text{atoms}}{\text{cm}^3}$$

$$N_D = \frac{0.015}{100} N_H = 0.00001029x10^{24}\frac{\text{atoms}}{\text{cm}^3}$$

Number density using weight percent

- Sometimes compositions are given in terms of percent of weight of the various constituents
- If ρ is the physical density of the mixture, then the density of an individual component is $\frac{\rho w_i}{100}$, where w_i is the weight percent (often abbreviated w/o) of component i
- The atom density of this component is $N_i = \frac{w_i \rho N_A}{100 A_i}$
- A reactor is fueled with Uranium enriched to 20 w/o U235 and the rest U238. The density is 19.1 g/cc. The atomic weights of U235 and U238 are 235.0439 and 238.0508.

$$N_{U235} = \frac{20 * 19.1 \frac{\text{g}}{\text{cm}^3} * 0.6022x10^{24} \frac{\text{atoms}}{\text{mol}}}{100 * 235.0439 \frac{\text{g}}{\text{mol}}} = 0.00979x10^{24} \frac{\text{atoms}}{\text{cm}^3}$$

$$N_{U238} = \frac{80 * 19.1 \frac{\text{g}}{\text{cm}^3} * 0.6022x10^{24} \frac{\text{atoms}}{\text{mol}}}{100 * 238.0508 \frac{\text{g}}{\text{mol}}} = 0.0386x10^{24} \frac{\text{atoms}}{\text{cm}^3}$$

Calculating w/o and atomic weight of mixtures

- Given some compound $X_m Y_n$, the molecular weight is $m A_x + n A_y$. The weight percent of X is

$$w/o(X) = \frac{mA_x}{mA_x + nA_y} * 100$$

- To calculate the atomic weight

$$\frac{1}{A} = \frac{1}{100} \sum \frac{w_i}{A_i}$$

Final Example

- A reactor is fueled with UO_2 pellets with density 10.5 g/cc. The U is enriched to 30 w/o in U235, what is the atom density of U235 in the fuel?
- First compute atomic weight of U

$$\frac{1}{A_U} = \frac{1}{100}\left(\frac{30}{235.0439} + \frac{70}{238.0508}\right), \qquad A_U = 237.141$$

- Compute molecular weight of UO2

$$A_{UO2} = 237.141 + 2*159994 = 269.139$$

- Find w/o of Uranium

$$w/o(U) = \frac{237.141}{269.139}*100 = 88.1$$

- Find U235 density

$$\rho_U = 0.881*10.5 = 9.25\frac{\text{g}}{\text{cm}^3}$$

$$\rho_{U235} = 0.30*9.25 = 2.78\frac{\text{g}}{\text{cm}^3}$$

$$N_{U235} = \frac{2.78\frac{\text{g}}{\text{cm}^3}*0.6022x10^{24}\frac{\text{atoms}}{\text{mol}}}{235.0439\frac{\text{g}}{\text{mol}}} = 0.00711x10^{24}\frac{\text{atoms}}{\text{cm}^3}$$