24.331 Fundamentals of NSE

Lesson 4: Atomic & Nuclear Physics I

Basic Notation and Material Atom Densities

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See Chapter 1 in your text by Shultis & Faw

Lesson 4 Objectives

Describe the basic structure of the atom.

Describe the basic notation used to identify various nuclides.

Define the term relative atomic weight, M_r.

Define the term gram atomic weight, M.

Compute M for an element containing more than one isotope when the isotopic abundances, γ_i, are given in atom percent (a/o).

Compute M for a mixture of isotopes or elements when the component compositions, w_i, are given in weight percent (w/o).

Compute material atom densities within individual regions under a variety of situations.

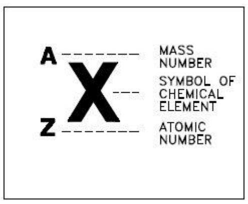
Lesson 4 Objectives

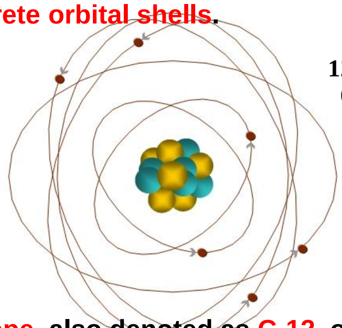
Compute material atom densities homogenized within a zone containing two or more discrete material regions.

Compare the relative volumes of the nucleus and atom and discuss the concept of the neutron field as a dilute gas within the “empty space”.

Structure of an Atom

The Bohr model of an atom has the nucleus containing the protons and neutrons in a compact central region surrounded by the electron cloud within discrete orbital shells.





$^{12}_{6}\mathrm{C}$

For example, the carbon-12 isotope, also denoted as C-12, or C12, has 6 protons (Z = 6), a mass number of 12 (A = 12), and 6 neutrons (N = A - Z = 6). The neutral atom also has 6 electrons to balance the positive charge of the 6 protons.

The Standard Model

Although we will focus on the **Bohr model** of an atom in this course, with its primary focus on **protons, neutrons, and electrons** as the **fundamental building blocks** of the atom, you should also be aware that there are a number of **subatomic particles** that interact to form the **nucleons within the Bohr atom**.

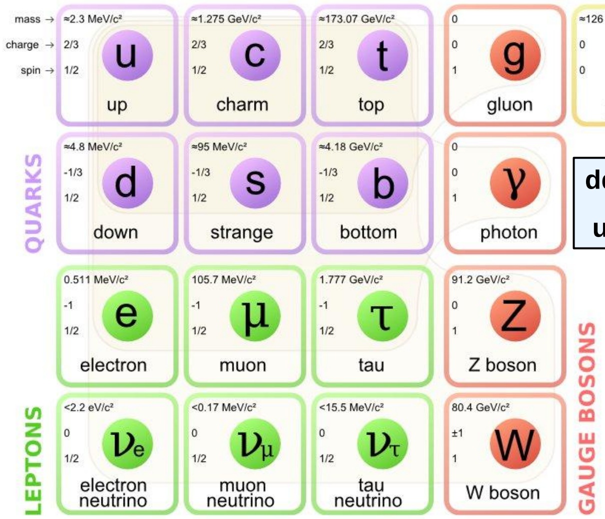
In particular, the **Standard Model of particle physics** describes the universe in terms of **matter** (**fermions**) and **force** (**bosons**).

There are **17 fundamental particles** identified to date: **6 quarks** (**fermions**), **6 leptons** (**fermions**), **4 force-carrying particles** (**gauge bosons**), and the **Higgs boson** (**see next slide**).

All the **matter particles** (**fermions**) have associated **antimatter particles** with the **same mass** but **opposite sign**.

Matter and antimatter interactions of the same type **annihilate matter to produce energy** -- that is, force particles (**bosons**) .

The Standard Model (cont.)



$ddu + g \rightarrow$ neutron

$uud + g \rightarrow$ proton

The Standard Model (cont.)

KNOWN FORCES (Gauge bosons)

FORCE	PARTICLE /QUANTUM	RELATIVE STRENGTH	MASS (GeV)	RANGE (meters)
Strong nuclear	gluon	1	0.14 (?)	10^{-15}
Electromagnetic	photon	7 X 10^{-3}	none	infinite
Weak nuclear	W^{+},W^{-} & Z bosons	10^{-5}	80-90	10^{-17}
Gravitation	gravitron (tentative)	6 X 10^{-39}	none	infinite

Particle physics is absolutely fascinating stuff!!!

However, for most practical applications, this level of theoretical understanding (i.e. the Standard Model) is not necessary -- so, to keep our discussions of NSE relatively straightforward, we will retain the simple idea that the neutrons, protons, and electrons are the fundamental building blocks of the atom…

Some Terminology

So, from our perspective, atoms consist of protons and neutrons (both are considered nucleons) within the nucleus, with the electrons within shells or orbits that surround the nucleus!!!

The number of protons, Z, defines the element.

A neutral atom will also have Z electrons.

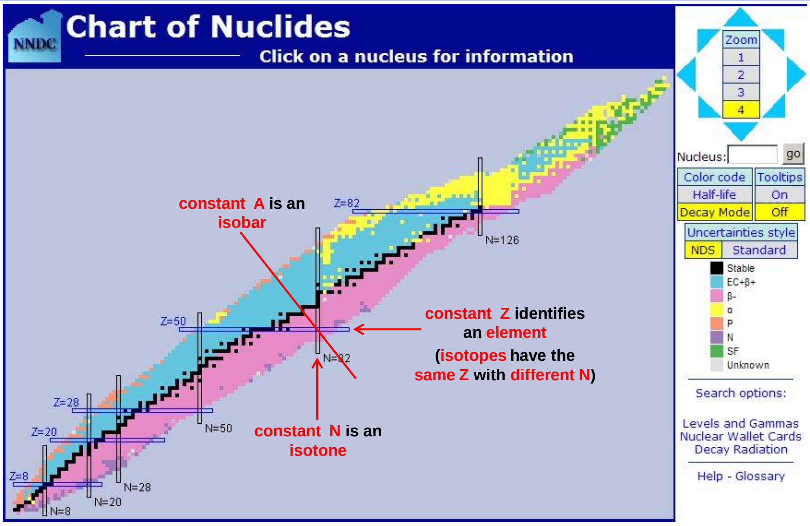
Isotopes have the same Z and different N.

An isobar includes nuclides with constant A.

An isotone consists of all nuclides with a common N.

These terms can be illustrated quite nicely on a Chart of the Nuclides (see next slide)…

Some Terminology (cont.)



Atomic Mass Unit

A mole is the amount of a substance which contains as many elementary entities as there are atoms in 12 grams of C-12, and there are $N_A \approx 0.602214\times10^{24}$ atoms in 12 grams of C-12.

Of course, you know N_A as Avogadro's number and this means that a mole of anything contains $N_A \approx 0.6022\times10^{24}$ entities of the quantity of interest (atoms or molecules in our case).

$$m\left({}^{12}_{6}\mathrm{C}\right) = \text{mass of 1 atom of } {}^{12}\mathrm{C} = \frac{12\,\text{g of } {}^{12}\mathrm{C}}{0.602214\times10^{24}\,\text{atoms of } {}^{12}\mathrm{C}}$$

The atomic mass unit or amu is defined as the mass associated with 1/12^th^ the mass of a single C-12 atom.

$$1\,\text{amu} = \frac{1}{12}\times\left(\text{mass of 1 atom of } {}^{12}\mathrm{C}\right) = \frac{1}{N_A}\,\text{g} = \frac{1}{0.602214\times10^{24}}\,\text{g} = 1.66054\times10^{-24}\,\text{g}$$

numerically, 1 amu = $1/N_A$

Atomic or Molecular Weight

The formal definition for the atomic weight (M_r) of an atom or the molecular weight of a molecule is given in terms of the ratio of the mass of the neutral atom or molecule relative to 1/12th the mass of a neutral C-12 atom (M_r is a dimensionless number).

$$M_{ri} = \frac{\text{mass of 1 atom of isotope i}}{\text{mass of } \frac{1}{12} \text{ of the } {}^{12}\text{C atom}}$$

The gram atomic weight (M) is defined as the mass of one mole of a substance (M has units of g/gmole).

$$M_i = m(X_i)\times N_A = M_{ri}\times\left(\text{mass of } \tfrac{1}{12} \text{ of the } {}^{12}\text{C atom}\right)\times N_A = M_{ri}\times\left(\frac{1}{N_A}\text{g}\right)\times N_A = M_{ri}\,\text{g}$$

In our work, we will always use the terms atomic or molecular weight to mean the gram atomic weight with units of g/gmole -- and this is simply interpreted as the mass (in grams) of one mole (N_A atoms) of a particular nuclide or molecule.

Molecular Weight of Mixtures

The molecular weight of a molecule is merely the sum of the atomic weights of its constituents.

For example, the molecular weight of water (H_2O) is given by

$$M_{H_2O} = 2\times M_H + M_O = 2\times(1.00797) + (15.9994) = 18.0153\text{ g/gmole}$$
$$\approx 2\times(1) + (16) = 18\text{ g/gmole}$$

The atomic weight of an element having more than one isotope is given by

$$M = \sum_i \gamma_i M_i = \sum_i \left(\frac{\text{atoms of i}}{\text{total atoms}}\right)\left(\frac{\text{g of i/gmole}}{N_A \text{ atoms of i/gmole}}\right) = \frac{\text{g of element}}{N_A \text{ atoms of element}}$$

For example, for natural boron, we have

$M_{Nat\,B}$ = (0.199)(10.0129) + (0.801)(11.0093)

= 10.811 g/gmole

i	γ_i (a/o)	M_i
^{10}B	19.9	10.0129
^{11}B	80.1	11.0093

Material Atom Densities

If one is given the mass density, ρ, of the material, then the material atom density, N, is given by

$$N = \frac{\left(\rho\ \mathrm{g/cm^3}\right)\left(N_A\ \mathrm{atoms/gmole}\right)}{M\ \mathrm{g/gmole}} = \frac{\rho N_A}{M}\,\frac{\mathrm{atoms}}{\mathrm{cm^3}}$$

If several isotopes are present and their abundances (a/o) are known,

$$N_i = \frac{\gamma_i \rho N_A}{M} = \gamma_i N$$

If the chemical composition of a mixture or element is given in terms of weight percent (w/o),

$$N_i = \frac{\rho_i N_A}{M_i} = \frac{w_i \rho N_A}{M_i}$$

Molecular Weight of a Mixture

In performing density computations, one often needs the molecular weight of the mixture.

If the components are given as atom fractions: $M = \sum_i \gamma_i M_i$

If the components are given as weight fractions: $\frac{1}{M} = \sum_i \frac{w_i}{M_i}$

Note:

The latter result can be obtained from

$$N = \frac{\rho N_A}{M} = \sum_i N_i = \sum_i \frac{w_i \rho N_A}{M_i}$$

after cancelling ρN_A when equating the second and fourth terms.

Example: Material Densities for UO_2

Given that the **density of uranium dioxide (UO_2) is 10.5 g/cm^3** and that the weight percent of **U235 is 4.2 w/o**, **calculate the atom densities of U235, U238, and O** in this fuel material.

Let's first find the **molecular weights of U and UO_2**. From above, we have

$$\frac{1}{M_U} = \sum_i \frac{w_i}{M_i} = \frac{0.042}{235} + \frac{0.958}{238} = 0.004204 \quad \text{or} \quad M_U = 237.9\,\text{g/gmole}$$

Thus, the **molecular weight of UO_2** becomes

$$M_{UO_2} = M_U + 2M_O = 237.9 + 32 = 269.9\ \text{g/gmole}$$

Now, **working with units to go from the given mass density to the desired atom density** gives,

$$\frac{10.5\,\text{g of UO}_2}{\text{cm}^3} \times \frac{237.9\,\text{g of U}}{269.9\,\text{g of UO}_2} \times \frac{0.042\,\text{g of U235}}{\text{g of U}} \times \frac{0.6022\times 10^{24}\ \text{at. of U235}}{235\,\text{g of U235}}$$

Example: Material Densities for UO_2

or

$$N_{U235} = 9.961\times 10^{20}\ \frac{\text{at. of U235}}{\text{cm}^3}$$

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Note: Before continuing we note that, in the **NSE arena**, the atom densities are usually expressed in units of **atoms/b-cm**, where **1 b = 1 barn = 10^{-24} cm^2**, since the density usually multiplies the **microscopic cross section**, σ, to give the **macroscopic cross section**, $\Sigma = N\sigma$, and **σ is expressed in units of barns**. With these units we have

$$\Sigma = N\sigma \ \Rightarrow\ \frac{\text{atoms}}{\text{b-cm}} \times \text{b} = \frac{\text{atoms}}{\text{cm}} = \text{cm}^{-1}$$

$\mu = N\sigma$ is used for photons
(linear interaction coeff.)

Putting N_{U235} into these units gives

$$N_{U235} = 9.961\times 10^{20}\ \frac{\text{at. of U235}}{\text{cm}^3} \times \frac{10^{-24}\ \text{cm}^2}{\text{b}} = 9.961\times 10^{-4}\ \frac{\text{at. of U235}}{\text{b-cm}}$$

Example: Material Densities for UO_2

Now, using the same approach as above, the atom densities for U238 and O become

$$N_{U238} = (10.5)\left(\frac{237.9}{269.9}\right)(0.958)\left(\frac{0.6022}{238}\right) = 2.243\times10^{-2}\ \frac{\text{at. of U238}}{\text{b-cm}}$$

$$N_{O} = (10.5)\left(\frac{32}{269.9}\right)\left(\frac{0.6022}{16}\right) = 4.686\times10^{-2}\ \frac{\text{at. of O}}{\text{b-cm}}$$

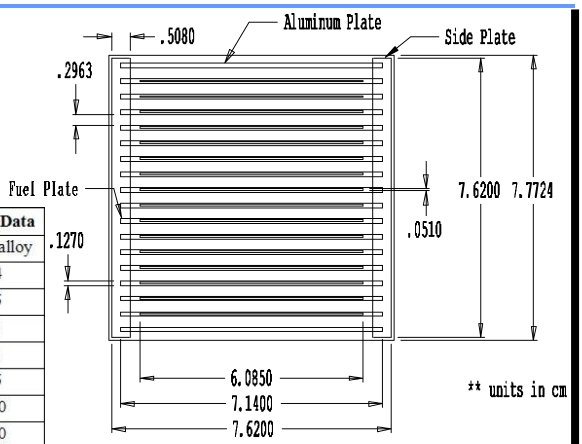
As a check, we know that the ratio of O atoms to U atoms should be 2, thus

$$N_{O} = 2N_{U} = 2(N_{U235}+N_{U238}) = 2\left(9.961\times10^{-4}+2.243\times10^{-2}\right) = 4.685\times10^{-2}\ \frac{\text{at of O}}{\text{b-cm}}$$

This check gives the above result (to within round-off error).

Example: UMLRR Fuel Meat Material Densities

Data for the LEU Fuel Plate



LEU Fuel Plate Geometry + Composition Data	
fuel type	U_3Si_2-Al alloy
U_3Si_2 fraction (w/o)	67.54
U235 enrichment fraction (w/o)	19.75
U235 loading (g/plate)	12.5
plate width (cm)	7.14
fuel meat width (cm)	6.085
plate thickness (cm)	0.1270
fuel meat thickness (cm)	0.0510
plate height (cm)	63.5
fuel meat height (cm)	59.69
fuel meat volume (cm^3)	18.524

Example: UMLRR Fuel Meat Material Densities

Given the fuel supplier's data for the LEU fuel plate geometry and composition, calculate the atom densities of U235, U238, Si, and Al in the central fuel meat region.

Let's first compute the mass density of U235 within the fuel meat

$$\rho_{U235} = \frac{12.5\,g}{plate} \times \frac{plate}{18.524\,cm^3} = 0.6748\,g/cm^3$$

Now

$$N_{U235} = \frac{\rho_{U235} N_A}{M_{U235}} = \frac{0.6748\,g}{cm^3}\,\frac{0.6022\,at.\,cm^2/b}{235.04\,g} = 1.729\times10^{-3}\,\frac{at.\,U235}{b\text{-}cm}$$

With the U235 density and enrichment, we can compute the total U density and the U238 density, as follows:

$$\rho_U = \frac{0.6748\,g\,U235}{cm^3}\,\frac{1\,g\,U}{0.1975\,g\,U235} = 3.417\,g\,U/cm^3$$

Example: UMLRR Fuel Meat Material Densities

$$\frac{1}{M_U} = \sum_i \frac{w_i}{M_i} = \frac{0.1975}{235.04} + \frac{0.8025}{238.05} = 0.004211 \quad \text{or} \quad M_U = 237.45\,g/gmole$$

$$N_U = \frac{3.417\,g}{cm^3}\,\frac{0.6022\,at.\,cm^2/b}{237.45\,g} = 8.666\times10^{-3}\,\frac{at.\,U}{b\text{-}cm}$$

and $$N_{U238} = N_U - N_{U235} = 6.937\times10^{-3}\,\frac{at.\,U238}{b\text{-}cm}$$

Since each U_3Si_2 molecule has two atoms of silicon and three atoms of uranium, we have

$$N_{U_3Si_2} = \frac{1}{3}N_U = \frac{1}{2}N_{Si}$$

and $$N_{Si} = \frac{2}{3}N_U = \frac{2}{3}\left(8.666\times10^{-3}\right) = 5.777\times10^{-3}\,\frac{at.\,Si}{b\text{-}cm}$$

Example: UMLRR Fuel Meat Material Densities

Finally, knowing the U_3Si_2 fraction, we can compute the aluminum density within the fuel meat as follows:

$$M_{U_3Si_2} = 3M_U + 2M_{Si} = 3(237.45) + 2(28.086) = 768.52 \quad \text{g/gmole}$$

$$\rho_{Al} = \frac{3.417\,\text{g of U}}{\text{cm}^3} \times \frac{768.52\,\text{g of } U_3Si_2}{3(237.45)\,\text{g of U}} \times \frac{(1-0.6754)\,\text{g of Al}}{0.6754\,\text{g of } U_3Si_2} = 1.7717\,\text{g Al/cm}^3$$

and $$N_{Al} = \frac{1.7717\,\text{g}}{\text{cm}^3}\,\frac{0.6022\,\text{at. cm}^2/\text{b}}{26.982\,\text{g}} = 3.954\times10^{-2}\,\frac{\text{at. Al}}{\text{b-cm}}$$

Thus, the desired atom densities for the fuel meat within the LEU fuel plate are:

$$\boxed{\begin{array}{ll} N_{U235} = 1.729\times10^{-3}\,\dfrac{\text{at. U235}}{\text{b-cm}} & N_{U238} = 6.937\times10^{-3}\,\dfrac{\text{at. U238}}{\text{b-cm}} \\ N_{Si} = 5.777\times10^{-3}\,\dfrac{\text{at. Si}}{\text{b-cm}} & N_{Al} = 3.954\times10^{-2}\,\dfrac{\text{at. Al}}{\text{b-cm}} \end{array}}$$

Homogenized Material Densities

Discrete heterogeneous material regions are often assumed to be mixed homogeneously to give a macroscopic zone with constant material properties.

This procedure is valid if the average distance traveled by the neutron is greater than the dimensions of the discrete hetero-geneous regions.

When this occurs the whole group of regions appear as a quasi-homogeneous mixture with essentially constant properties.

To compute densities averaged over a zone containing multiple discrete regions, we simply multiply the region densities by the region volume fraction within the zone and add the individual volume-weighted contributions.

Homogenized Material Densities

This can be represented mathematically as

$$\boxed{N_{iz} = \frac{\sum_{j\in z} N_{ij} V_j}{\sum_{j\in z} V_j} = \sum_{j\in z} N_{ij} f_j}$$

isotope i, region j, zone z

f_j = volume fraction of region j in zone z

For example, for a 2-region case:

$$N_i^{homo} = \left(\frac{\text{atoms of i}}{\text{cm}^3 \text{ of region 1}}\right)\left(\frac{\text{cm}^3 \text{ of region 1}}{\text{cm}^3 \text{ of total}}\right) + \left(\frac{\text{atoms of i}}{\text{cm}^3 \text{ of region 2}}\right)\left(\frac{\text{cm}^3 \text{ of region 2}}{\text{cm}^3 \text{ of total}}\right)$$

or

$$N_i^{homo} = N_{i1} f_1 + N_{i2} f_2$$

Example: Homogenized Densities -- PWR Fuel Pin

Consider a single 3-region fuel pin cell within a typical PWR 17×17 fuel assembly with the following data:

Composition:

Fuel: 4.2 w/o UO_2 at 10.5 g/cc

Clad: pure Zr at 6.56 g/cc

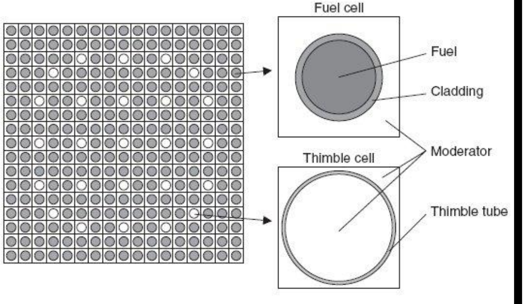
Moderator: water at 0.72 g/cc

Geometry:

Fuel OD: 0.9566 cm

Clad Thickness: 0.0572 cm

Pin Pitch: 1.25 cm



Example: Homogenized Densities -- PWR Fuel Pin

Compute the region atom densities and the cell-averaged densities for the homogenized fuel/clad/moderator fuel pin cell.

Region Densities:

Fuel: $N_{U235} = 9.961\times10^{-4}\ \frac{\text{at.}}{\text{b-cm}}$ $\quad N_{U238} = 2.243\times10^{-2}\ \frac{\text{at.}}{\text{b-cm}}$

$N_O = 4.686\times10^{-2}\ \frac{\text{at.}}{\text{b-cm}}$ **(from previous example)**

Clad: $N_{Zr} = \frac{6.56\,g}{cm^3}\ \frac{0.6022\,\text{at. cm}^2/\text{b}}{91.22\,g} = 4.331\times10^{-2}\ \frac{\text{at.}}{\text{b-cm}}$

Moderator: $N_{water} = \frac{0.72\,g}{cm^3}\ \frac{0.6022\,\text{molecules cm}^2/\text{b}}{18\,g} = 2.409\times10^{-2}\ \frac{\text{molecules}}{\text{b-cm}}$

Example: Homogenized Densities -- PWR Fuel Pin

Region Volume Fractions:

- **total cell volume** = (1.25 cm)(1.25 cm) = 1.5625 cm^2
- **fuel pin volume** = (π/4)(0.9566 cm)^2 = 0.7187 cm^2
- **clad volume** = (π/4)((0.9566 + 2*0.0572) cm)^2 – 0.7187 cm^2 = 0.1822 cm^2
- **water volume** = 1.5625 cm^2 – (0.7187 + 0.1822) cm^2 = 0.6616 cm^2

With these data, the **volume fraction for region j is given by V_j/V_{total}**:

Region Volume Fractions

Region	Volume Fraction
fuel	0.4600
clad	0.1166
water	0.4234

Example: Homogenized Densities -- PWR Fuel Pin

Cell-Averaged Homogenized Densities:

We can compute the desired homogenized densities by simply multiplying the region densities and the region volumes fractions from above, with a sum over regions if the same nuclide appears in multiple regions (this latter step is not needed here).

Doing this gives the number of atoms of each isotope/material per unit cell volume:

Cell Averaged Atom Densities (atoms/b-cm).

Material	Average Density
U235	4.582e-4
U238	1.032e-2
O	2.156e-2
Zr	5.050e-3
H_2O	1.020e-2

Relative Size of the Nucleus and Atom

The size of the atom is difficult to specify precisely because the electron cloud does not have a definite edge.

However, except for the lightest atoms, the average atomic radii are approximately constant at about 2×10^{-8} cm, which gives a spherical volume of about 3×10^{-23} cm^3 (which is indeed a very small volume).

The nucleus, containing the protons and neutrons in the center of the atom, is also somewhat spherical in shape with a radius given by

$$R = 1.25\times10^{-13}\,A^{1/3}\ \text{cm}$$

Using this expression, the volume of the nucleus is about 8×10^{-39} A cm^3, which for the largest A, only gives about 2×10^{-36} cm^3 (and this is an exceeding small volume -- absolutely minuscule compared to the volume of a single atom).

Relative Size of the Nucleus and Atom

Thus, the atom is essentially "empty space", except for a very tiny nucleus and for the electrons orbiting this tiny nucleus.

We also note that typical neutron densities in a nuclear reactor core are on the order of about $10^7 - 10^9$ neutrons/cm^3 and that typical atom densities are on the order of $10^{20} - 10^{22}$ atoms/cm^3.

Thus, the neutron population is extremely small relative to the population of material atoms that make up the reactor core.

But, since atoms are essentially "empty space", we can visualize the neutrons as a very dilute gas that moves through this "empty space", with some occasional interaction of the neutrons with the target nuclei that make up the background material.

We will use this "view" of the neutron field in later discussions of neutron transport and diffusion within the background material media.

Lesson 4 Summary

In this Lesson we have briefly discussed the following subjects:

The basic structure of the atom and the notation used to identify nuclides.

The difference between the terms relative atomic weight, M_r, and gram atomic weight, M.

The computation of M for an element containing more than one isotope when the isotopic abundances, γ_I are given.

The computation of M for a mixture of isotopes or elements when the component compositions, w_i, are given.

The computation of material atom densities within individual regions under a variety of situations.

Lesson 4 Summary

The computation of material atom densities homogenized within a zone containing two or more discrete material regions.

The relative volumes of the nucleus and atom and the concept of the neutron field as a dilute gas within the "empty space".