Team Exercise Solutions #2

Problem 1

Compute the atomic densities of ^{235}U, ^{238}U, and O in UO_2 when its density is 10.41 g/cm^3 and the uranium is enriched to 5 wt% in ^{235}U.

Problem 1 Solution

First, let's note that we will use the shorthand U5 and U8 in subscripts to denote ^{235}U and ^{238}U respectively.

To begin we note that the densities of ^{235}U and ^{238}U can be found as fractions of the total UO_2. Since the partial densities are dependent on the mass of the components, the fractions are equivalent to the weight % enrichment.

$$\rho_{\mathrm{UO_2}} = \rho_{\mathrm{U5O_2}} + \rho_{\mathrm{U8O_2}}$$

$$\begin{aligned} \rho_{\mathrm{U5O_2}} &= w\rho_{\mathrm{UO_2}} \\ \rho_{\mathrm{U8O_2}} &= (1-w)\rho_{\mathrm{UO_2}} \end{aligned} \quad \text{where } w = 0.05$$

Now, we can use the fact that the number density of a material, n, is equal to the material's density, ρ, multiplied by Avogadro's number, N_A, and divided by the molar mass, m, of the material.

$$n = \frac{\rho N_A}{m}$$

We find

$$n_{\mathrm{U5O_2}} = \frac{\rho_{\mathrm{U5O_2}} N_A}{m_{\mathrm{U5O_2}}}$$

$$n_{\mathrm{U8O_2}} = \frac{\rho_{\mathrm{U8O_2}} N_A}{m_{\mathrm{U8O_2}}}$$

If we make the simplification that $n_{\mathrm{U5}} = n_{\mathrm{U5O_2}}$ and $n_{\mathrm{U8}} = n_{\mathrm{U8O_2}}$, and also substitute our equations for $\rho_{\mathrm{U5O_2}}$ and $\rho_{\mathrm{U8O_2}}$ in terms of $\rho_{\mathrm{UO_2}}$ from above, then we find

$$n_{\mathrm{U5}} = \frac{w\rho_{\mathrm{UO_2}} N_A}{m_{\mathrm{U5O_2}}}$$

$$n_{\mathrm{U8}} = \frac{(1-w)\rho_{\mathrm{UO_2}} N_A}{m_{\mathrm{U8O_2}}}$$

At this point, we can also separate our molar masses into molar masses of the components, for which we can find data.

$$m_{\mathrm{U5O_2}} = m_{\mathrm{U5}} + 2m_{\mathrm{O}}$$

$$m_{\mathrm{U8O_2}} = m_{\mathrm{U8}} + 2m_{\mathrm{O}}$$

We now have enough information to solve for both of these quantities, and so we plug in values. We also note that $n_O = 2(n_{\mathrm{U8}} + n_{\mathrm{U8}})$ since each uranium atom is bonded to 2 oxygen atoms.

$$n_{\mathrm{U5}} = \frac{w\rho_{\mathrm{UO_2}} N_A}{m_{\mathrm{U5}} + 2m_{\mathrm{O}}} \qquad \boxed{n_{\mathrm{U5}} = 1.174 \times 10^{21}\ \mathrm{cm^{-3}}}$$

$$n_{\mathrm{U8}} = \frac{(1-w)\rho_{\mathrm{UO_2}} N_A}{m_{\mathrm{U8}} + 2m_{\mathrm{O}}} \qquad \boxed{n_{\mathrm{U8}} = 2.205 \times 10^{22}\ \mathrm{cm^{-3}}}$$

$$n_{\mathrm{O}} = 2(n_{\mathrm{U5}} + n_{\mathrm{U8}}) \qquad \boxed{n_{\mathrm{O}} = 4.645 \times 10^{22}\ \mathrm{cm^{-3}}}$$

Problem 2

Free neutrons undergo β^- decay with a half-life of 10.4 minutes. Determine the probability that a neutron will decay before being absorbed in an infinite absorbing material (assume no scattering). Estimate this probability for a thermal neutron ($v = 2200$ m/s) in water.

Problem 2 Solution

Since we are assuming no scattering, at any given time t there are three possible "fates" of our neutron in the next infinitesimal timestep, dt. These are (1) the particle continues with no decay or interaction, (2) the neutron decays, or (3) the neutron is absorbed. We want to find the probability that, given a destructive event has taken place (situation 2 or 3), the event was decay, rather than absorption. Formally, we write this as

$$\mathrm{p}(E = d | E \in \{d, a\})$$

which we read as "the instantaneous probability that an event is decay, given the event was decay or absorption." Statistically this is equivalent to

$$\frac{\mathrm{p}(E = d)}{\mathrm{p}(E \in \{d, a\}} \text{ or } \frac{\mathrm{p}(d)}{\mathrm{p}(d) + \mathrm{p}(a)}. \tag{1}$$

(If you're not comfortable with the statistics here, you can reason through this intuitively. We have some event occuring, being either a decay or an absorption collision. The probability of that event depends on the individual probabilities of the independent events, decay and absorption. The probability of that event being a decay is just the fraction of the event's total probability that is attributable to the decay.)

From here on, we will write the argument of the probality function as a subscript, which will allow us to note the probability's dependence on either time or space. (For example, $\mathrm{p}(d) \rightarrow \mathrm{p}_d$.)

Now, we know that the exponential decay law is $N(t) = N_0 e^{-\lambda t}$. The probability that a neutron decays in some time t is then

$$P_d(t) = 1 - \frac{N(t)}{N_0} = 1 - e^{-\lambda t}$$

We can calculate that the instantantaneous probability that a neutron decays between times t and $t + dt$ is

$$\frac{dP_d(t)}{dt} = \lambda e^{-\lambda t}$$

From this equation, we note that $dP_d(t) = p_d(t)dt$. Remember, $P_d(t)$ is the total probability of decay, and so $p_d(t)$ is the instantaneous probability of decay per time. When multiplied by dt, this is $\mathrm{p}_d(t)$.

$$\mathrm{p}_d(t) = p_d(t)\, dt = \lambda e^{-\lambda t} dt$$

We rewrite this equation in terms of $N(t)$, and

$$\mathrm{p}_d(t) = \frac{\lambda N(t)}{N_0} dt$$

Additionally, we know that the attenuation of neutrons moving through a material also follows an exponential function. The number of neutrons remaining after traveling through a material with macroscopic absorption cross section Σ_a, is

$$N(x) = N_0 e^{-\Sigma_a x}$$

(note: $\Sigma_a = \sigma_a n$, where σ_a is the microscopic absorption cross section and n is the number density of the material in question)

We repeat the procedure from above, but now in space rather than time. The probability for a collision is

$$P_a(x) = 1 - \frac{N(x)}{N_0} = 1 - e^{-\Sigma_a x}$$

and the instantaneous probability is

$$\frac{dP_a(x)}{dt} = \Sigma_a e^{\Sigma_a x}$$

or

$$\mathrm{p}_a(x) = p_a(x)\,dx = \Sigma_a e^{\Sigma_a x} dx.$$

Again, eliminating dx and writing in terms of $N(x)$, we have

$$\mathrm{p}_a(x) = \frac{\Sigma_a N(x)}{N_0} dx$$

Now, we observe that using $\mathrm{p}_d(t)$ and $\mathrm{p}_a(x)$ in equation (1) causes all terms to be dependent on N, the number of neutrons. Unfortunately, we have p_d reliant on $N(t)$, the number of neutrons surviving until time t, and p_a reliant on $N(x)$, the number of neutrons reaching distance x. We are told, however, that these neutrons are thermal, and so are moving at $v = 2200$m/s. If we say $dx = v\,dt$, then we can rewrite $N(x)dx$ as a function of time!

$$N(x)\,dx = N(t)v\,dt$$

and

$$\mathrm{p}_a(t) = \frac{\Sigma_a N(t)v}{N_0} dt$$

Finally, we do substitute this into equation (1), and get

$$\begin{aligned} \mathrm{p}(E = d | E \in \{d, a\}) &= \frac{\frac{\lambda N(t)}{N_0} dt}{\frac{\lambda N(t)}{N_0} dt + \frac{\Sigma_a N(t) v}{N_0} dt} \\ &= \frac{\lambda}{\lambda + \Sigma_a v} \\ &= \left(1 + \frac{\Sigma_a v}{\lambda}\right)^{-1} \end{aligned}$$

We can look up Σ_a to find it is approximately 0.022 cm^{-1} (or 2.2 m^{-1}, and can calculate that 10.2 minutes is 612 seconds. Using this, along with $v = 2200$ m/s, and $\lambda = \frac{\ln 2}{612} = 1.13 \times 10^{-3}$ s^{-1}, we can find the probability.

$$\mathrm{p}(E = d | E \in \{d, a\}) = \left(1 + \frac{(2.2 \text{ m}^{-1})(2200 \text{ m/s})}{1.13 \times 10^{-3} \text{ s}^{-1}}\right)^{-1}$$

$$\boxed{\mathrm{p}(E = d | E \in \{d, a\}) = 2.33 \times 10^{-7}}$$

Problem 3

Consider a 1000 MWE reactor with a 33% efficiency conversion from MWT to MWE. What is the minimum volume of UO_2, enriched to 3 (atom) % ^{235}U that could theoretically supply the yearly energy production of this reactor. Treat energy contributions as coming only from the fission of ^{235}U. These fission events release about 200 MeV with 95% of that energy staying in the reactor.

Problem 3 Solution

We need to find the minimum required volume of UO_2, V, so let's begin by expressing that volume of UO_2 in terms of the number of UO_2 molecules it contains.

First, we use M_{UO_2} as the total mass of UO_2 and ρ_{UO_2} as the density of UO_2 (about 10.41 g/cm^3 for our purposes)

$$V = \frac{M_{\mathrm{UO}_2}}{\rho_{\mathrm{UO}_2}}$$

Then, we can write the mass of UO_2 as the number of UO_2 molecules, N_{UO_2}, times the mass of a UO_2 molecule, m_{UO_2}. Since we know that the UO_2 is enriched such that 3% of the molecules contain ^{235}U, we can say $m_{\mathrm{UO}_2} = 0.03m_{\mathrm{U5}} + 0.97m_{\mathrm{U8}} + 2m_{\mathrm{O}}$. Then

$$M_{\mathrm{UO}_2} = N_{\mathrm{UO}_2}(0.03m_{\mathrm{U5}} + 0.97m_{\mathrm{U8}} + 2m_{\mathrm{O}})$$

We can use this equality in our total volume equation to find

$$V = \frac{N_{\mathrm{UO}_2}(0.03m_{\mathrm{U5}} + 0.97m_{\mathrm{U8}} + 2m_{\mathrm{O}})}{\rho_{\mathrm{UO}_2}} \tag{2}$$

Now we need to relate this volume, in terms of number of UO_2 molecules, to the electric power produced by the reactor. Say P_E is the electric power, P_T is thermal power, and ε is the efficiency.

$$P_E = \varepsilon P_T$$

The total energy produced by the reactor in time t can be found by simply multiplying the power by the time of production.

$$E = P_T t$$

or equivalently

$$P_T = \frac{E}{t}.$$

The energy from one fission is E_f and the energy harnessed from one fission is $0.95E_f$. The total energy harnessed can then be expressed in terms of the number of fissions, N_f and the energy captured per event,

$$E = 0.95E_f N_f$$

If we consider the extreme and highly unrealistic case that *all* ^{235}U atoms fission, then the number of ^{235}U atoms required is $N_{\mathrm{U5}} = N_f$. Since ^{235}U is 3% of the total uranium by atom, then $N_{\mathrm{U5}} = 0.03N_{\mathrm{U}}$. Taking this one step further, there is a one-to-one ratio of uranium atoms to UO_2 molecules, so $N_{\mathrm{U}} = N_{\mathrm{UO}_2}$.

We combine these facts together to relate the electric power produced to the number of uranium dioxide molecules required.

$$\begin{aligned} P_E &= \varepsilon P_T \\ &= \varepsilon \frac{E}{t} \\ &= \frac{0.95\varepsilon E_f N_f}{t} \\ &= \frac{(0.95)(0.03)\varepsilon E_f N_{\mathrm{UO}_2}}{t} \end{aligned}$$

We solve for $N_{\mathrm{UO_2}}$ to get

$$N_{\mathrm{UO_2}} = \frac{P_E t}{(0.95)(0.03)\varepsilon E_f} \tag{3}$$

Now, we use equation (3) for the number of $\mathrm{UO_2}$ molecules required for the given power in equation (2) for the volume of $\mathrm{UO_2}$ required. We find

$$V = \frac{P_E t(0.03 m_{\mathrm{U5}} + 0.97 m_{\mathrm{U8}} + 2 m_{\mathrm{O}})}{(0.95)(0.03)\varepsilon E_f \rho_{\mathrm{UO_2}}}$$

Finally, we can include our values. We note the following

- $P_E = 1000$ MWE $= 10^9$ J/s
- $t = 1$ yr $= 31,557,600$ s
- $E_f = 200$ MeV $= 3.204 \times 10^{-11}$ J
- $m_{\mathrm{U5}} = 235.044$ amu $= 3.9028 \times 10^{-22}$ g
- $m_{\mathrm{U8}} = 238.051$ amu $= 3.9528 \times 10^{-22}$ g
- $m_{\mathrm{O}} = 15.995$ amu $= 2.656 \times 10^{-23}$ g

$$V = \frac{(10^9\ \mathrm{J/s})(31557600\ \mathrm{s})(0.03(3.9028 \times 10^{-22}\ \mathrm{g}) + 0.97(3.9528 \times 10^{-22}\ \mathrm{g}) + 2(2.656 \times 10^{-23}\ \mathrm{g}))}{(0.95)(0.03)(0.33)(3.204 \times 10^{-11}\ \mathrm{J})(10.41\ \mathrm{g/cm^3})}$$

$$\boxed{V = 4.51\ \mathrm{m^3}}$$

Problem 4

Given UO_2 with 2.5×10^{21} atoms/cm^3 of ^{235}U and 2.0×10^{22} atoms/cm^3 of ^{238}U, find the partial densities of ^{235}U, ^{238}U, and O, and determine the enrichment.

Problem 4 Solution

The number density of material i can be found using the formula

$$n_i = \frac{\rho_i N_A}{M_i}$$

where ρ_i is the partial density of material i, M_i is the molar mass of i, and N_A is Avogadro's number. We can reverse this formula to find the partial density of a material from the atomic density.

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

We can use this formula for the three isotopes we are considering. We also note the following:

- $n_{\text{O}} = 2(n_{\text{U5}} + n_{\text{U5}})$
- $M_{\text{U5}} = 235.04$ g/mol
- $M_{\text{U8}} = 238.05$ g/mol
- $M_{\text{O}} = 16.00$ g/mol

$$\rho_{\text{U5}} = \frac{n_{\text{U5}} M_{\text{U5}}}{N_A}$$

$$\rho_{\text{U5}} = \frac{(2.5 \times 10^{21} \text{ atoms/cm}^3)(235.04 \text{ g/mol})}{6.022 \times 10^{23} \text{ atoms/mol}}$$

$$\boxed{\rho_{\text{U5}} = 0.976 \text{ g/cm}^3}$$

$$\rho_{\text{U8}} = \frac{n_{\text{U8}} M_{\text{U8}}}{N_A}$$

$$\rho_{\text{U8}} = \frac{(2.0 \times 10^{22} \text{ atoms/cm}^3)(238.05 \text{ g/mol})}{6.022 \times 10^{23} \text{ atoms/mol}}$$

$$\boxed{\rho_{\text{U8}} = 7.91 \text{ g/cm}^3}$$

$$\rho_{\text{O}} = \frac{n_{\text{O}} M_{\text{O}}}{N_A}$$

$$\rho_{\text{O}} = \frac{2(n_{\text{U5}} + n_{\text{U5}}) M_{\text{O}}}{N_A}$$

$$\rho_{\text{O}} = \frac{2(2.25 \times 10^{22} \text{ atoms/cm}^3)(16.00 \text{ g/mol})}{6.022 \times 10^{23} \text{ atoms/mol}}$$

$$\boxed{\rho_{\text{O}} = 1.20 \text{ g/cm}^3}$$

The enrichment of ^{235}U is therefore $\frac{\rho_{\text{U5}}}{\rho_{\text{U5}} + \rho_{\text{U8}}} = 0.1098 \quad \Rightarrow \quad \boxed{10.98\%}$