22.01 Fall 2016, Quiz 1 Study Sheet

October 18, 2016

1 Basics of Physics, Kinematics, and Relativity

$$p = mv = \sqrt{2mT}; \qquad T = \frac{1}{2}mv^2 \tag{1}$$

where p is momentum, m is mass, v is velocity, and T is kinetic energy of a particle.

$$T_{\gamma} = \frac{hc}{\lambda} \tag{2}$$

where h is Planck's constant, c is the speed of light, and λ is the wavelength of the photon.

$$\frac{1}{\lambda_{transition}} = Ry\left(\frac{1}{n_{final}^2} - \frac{1}{n_{initial}^2}\right)$$
(3)

where n corresponds to the initial and final electron shell levels, depending on the subscript. The Rydberg energy is given as follows:

$$Ry_Z = \frac{Z^2 m_{e^-} e_c^4}{8\epsilon_0^2 h^3 c}$$
(4)

where Z is the number of protons in the nucleus, m_{e^-} is the rest mass of the electron (511 keV), e_c is the charge on the electron (1.6 × 10⁻¹⁹C), and ϵ_0 is the permittivity of a vacuum to allow electric field lines through it.

$$\gamma = \frac{1}{\sqrt{1 - \frac{v^2}{c^2}}} = \frac{m_{relativistic}}{m_0} \tag{5}$$

where γ represents the gamma factor for relativistic motion, and m_0 is the rest mass of the particle. It is used to compute the relativistic mass of a particle traveling at significant fractions (1% and higher) of the speed of light:

$$T_{total} = m_0 \gamma c^2; \qquad T_{kinetic} = (\gamma - 1) m_0 c^2 \tag{6}$$

Consider the limiting cases here. If a particle is at rest (v=0, $\gamma = 1$), then its kinetic energy is zero, and its mass is equal to its rest mass. If the particle is travelling at the speed of light, then $\gamma \to \infty$ and it becomes infinitely massive. It also takes an infinite amount of kinetic energy to get a particle with non-zero mass moving at the speed of light.

2 Nuclear Reactions and Energetics

A general nuclear reaction proceeds, and is written as follows:

$$i + I \to f + F + Q;$$
 $I(i, f) F$ (7)

where i and I represent the small and large initial particles, respectively, f and F represent the small and large final particles, respectively (which may not be the same ones), and Q is the energy consumed or liberated from the reaction. The last term shown is the shorthand form.

This Q value is expressible in terms of many things, stemming from conservation of total rest mass energy and kinetic energy of the reaction:

$$T_i + m_i c^2 + \mathcal{P}_I^{\bullet} + m_I c^2 = T_f + m_f c^2 + T_F + m_F c^2 \tag{8}$$

Separating the two sets of masses and energies to one side or the other of the equation, it can be written as follows:

$$m_i c^2 + m_I c^2 - m_F c^2 = T_f + T_F - T_i = Q$$
(9)

where it is assumed that the large, initial particle is at rest, unless we're in CERN or the large hadron collider or something.

The binding energy of a nucleus in MeV is analogous to the *work of separation* of its constituent nucleons, and can therefore be written as the difference between the masses in amu $-c^2$ of its individual nucleons and the assembled nucleus:

$$B.E. (A, Z) = [ZM_H + (A - Z)M_n - M(A, Z)]c^2$$
(10)

where BE is the binding energy, Z is the proton number, A is the total number of nucleons, M_p is the rest mass of the proton, M_n is the rest mass of the neutron, and M(A,Z) is the mass of the nucleus.

All masses and energies can be equivalently expressed in units of energy, such as keV or MeV. To convert between the two, use the following conversion factor:

$$M [MeV] = M [amu] \times \left[\frac{931.49 MeV}{amu - c^2}\right] c^2$$
(11)

Pro tip: Don't round masses in amu! All those digits really count.

The excess mass in amu is the difference in amu between the number of nucleons in a nucleus and its actual mass in amu:

$$\Delta = M\left(A, Z\right) - A \tag{12}$$

Note how the excess mass and the binding energy are *directly* related:

$$B.E.(A,Z) = [ZM_H + (A - Z)M_n - A - \Delta]c^2$$
(13)

A semi-empirical estimate of the mass of a nucleus can be found using the *liquid drop model* of the nucleus:

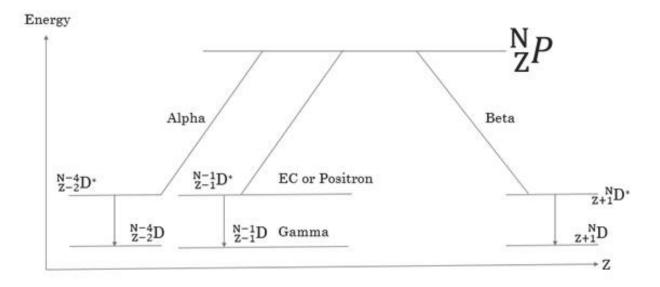
$$B.E.(A,Z) = a_v A - a_s A^{2/3} - a_c \frac{Z(Z-1)}{A^{1/3}} - a_a \frac{(A-2Z)^2}{A} + a_p \delta$$
(14)

For definitions of the terms, see the Yip book, p. 59, equation 4.10 and the following explanation.

3 Radioactive Decay

Spontaneous radioactive decay implies that Q>0, or that the reaction is exothermic. The opposite case would be when the reaction is *endothermic*, or would consume energy. The latter case requires additional energy to be imparted into the system to make the reaction move forward, just like in chemistry.

Below is a generalized radioactive decay diagram, showing all the potential daughter products (D) resulting from the decay of the same parent nuclide (P), courtesy of Ka-Yen Yau:



Spontaneous radioactive decay can proceed via a number of mechanisms, including:

3.1 Alpha (α) Decay

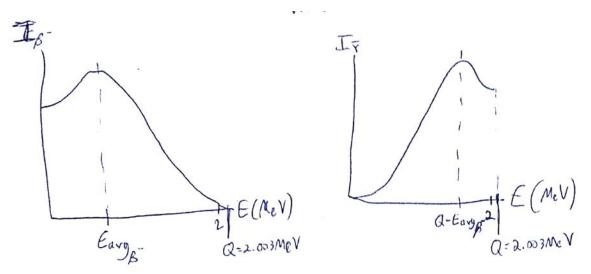
$${}^{A}_{Z}P \to {}^{A-4}_{Z-2}D + \alpha; \qquad Q[amu] = (M_P - M_D - M_\alpha)c^2$$
 (15)

Alpha particles are emitted monoenergetically, according to allowed transitions. Alpha decay may proceed to an excited state, which would allow further isomeric transitions (IT) or internal conversions (IC).

3.2 Beta (β^{-}) Decay

$${}^{A}_{Z}P \to^{A}_{Z+1}D + \beta^{-} + \bar{\nu}; \qquad Q[amu] = (M_P - M_D)c^2$$
 (16)

Betas and associated antineutrinos are emitted with a continuous spectrum, each having an average and maximum energy:



Beta decay may proceed to an excited state, which would allow further isomeric transitions (IT) or internal conversions (IC).

3.3 Positron (β^+) Decay

$${}^{A}_{Z}P \rightarrow^{A}_{Z-1}D + \beta^{+} + \nu; \qquad Q[amu] = (M_P - M_D - 2m_e)c^2$$
(17)

Positrons and associated neutrinos are emitted with a continuous spectrum, each having an average and maximum energy as above, though the intensity of positrons with zero energy begins at zero. Beta decay may proceed to an excited state, which would allow further isomeric transitions (IT) or internal conversions (IC). **Q must be above 1.022 MeV for this reaction to be allowable.** This is because in order to create a positron, and the associated, emitted electron (to conserve total charge), one must include two times the rest mass of the electron, 0.511MeV, just to create the particles necessary for this type of decay to occur.

3.4 Electron Capture (EC)

$${}^{A}_{Z}P \rightarrow^{A}_{Z-1} D; \qquad Q \left[amu\right] = \left(M_{P} - M_{D}\right)c^{2} - E_{Binding}$$
(18)

Instead of emitting a positron, the nucleus may capture an inner-shell electron, binding it with a proton to create a neutron. The inner-shell hole is then plugged by higher-energy electrons falling down in energy levels, emitting characteristic photons according to Equation 3. These also compete with the emission of Auger electrons, which may be ejected from outer shells.

3.5 Isomeric Transition (IT, γ Decay)

A nucleus in an excited state may decay by gamma ray emission to a lower energy state, which may or may not be the ground state:

$${}^{A}_{Z}P^{*} \rightarrow^{A}_{Z}P + \gamma; \qquad Q[MeV] = E_{\gamma}$$

$$\tag{19}$$

3.6 Internal Conversion (IC)

This process competes with IT, and involves the ejection of an inner-shell electron with an energy of $E_{e^-} = E_{\gamma} - E_{binding}$, with the latter given by Equation 3 with a final shell level of ∞ . This can also be followed by electron shell transitions with characteristic x-rays and/or Auger electrons as above.

3.7 Spontaneous Fission (SF)

Big nuclei just blow up sometimes. Even when it is energetically possible, the Q value needs to be high enough for the two nuclear pieces to overcome the strong nuclear force barrier and tunnel out of the nucleus. Needless to say it is a low-probability reaction, though it does happen for heavier nuclei:

$${}^{A}_{Z}P \to FP_1 + FP_2 + \eta_0^1 n; \qquad Q[amu] = (M(A,Z) - M_{FP_1} - M_{FP_1} - \eta M_n)c^2$$
 (20)

4 Allowable Nuclear Reactions and the Q-Equation

The full equation relating Q, the masses, energies, and angles involved in a general nuclear reaction are as follows:

$$T_f\left(1+\frac{M_f}{M_F}\right) - T_i\left(1-\frac{M_i}{M_F}\right) - \frac{2}{M_F}\sqrt{M_iM_fT_iT_f}\cos\theta \tag{21}$$

Reactions involving fewer particles can be simplified by setting appropriate terms to zero. There are a few important implications to this formula:

1. A necessary and sufficient condition for a reaction to proceed is that the sum of the kinetic energy of the incoming particle and the Q-value is positive:

$$T_i + Q \ge 0 \tag{22}$$

2. If a reaction is not allowed on its own (endothermic, Q<0), then there is a threshold energy required to induce it:

$$E_{threshold} = -Q \frac{M_f + M_F}{M_f + M_F - M_i} \approx -Q \frac{M_i + M_I}{M_I}$$
(23)

Note that energies are *always* positive, so for a reaction to have a threshold energy, it must be endothermic (Q<0).

3. For other implications, allowed angles, and energies, see Yip, pp. 142-149.

5 Radioactive Decay and Half Life

Activity is defined as follows:

$$A = \lambda N \tag{24}$$

where A is the activity in Bq (or Ci, remember that $1 \text{ Ci} = 3.7 \cdot 10^{10} \text{ Bq}$), λ is the decay constant in 1/s, and N is the number of decaying atoms present. Recognizing that:

$$A = -\frac{dN}{dt} \tag{25}$$

we can write:

$$\frac{dN}{dt} = -\lambda N \qquad \int \left(\frac{dN}{N}\right) = \int \left(-\lambda dt\right) \qquad \ln\left(N\right) = -\lambda t + C \qquad N\left(t=0\right) = N_0 \qquad N = N_0 e^{-\lambda t} \quad (26)$$

The half life $(t_{1/2})$ is solved by setting the fraction $\frac{N}{N_0}$ equal to 0.5:

$$t_{1/2} = \frac{\ln\left(2\right)}{\lambda} \qquad equivalently, \qquad \lambda = \frac{\ln\left(2\right)}{t_{1/2}} \tag{27}$$

6 Series Radioactive Decay

6.1 Core Concepts

The concentration of a particular isotope, or chain of isotopes, can always be written as the balance between production and destruction:

$$\frac{dN_i}{dt} = Prod_{\cdot i} - Destr_{\cdot i} \tag{28}$$

Production can either be directly from bombarded particles, or from another radioactive decay:

$$Prod._{i} = \underbrace{N_{i-1}\sigma_{capture_{i-1}}}_{like\ an\ "artificial\ \lambda"} \Phi + \lambda_{i-1}N_{i-1}$$
(29)

where σ is the *cross section*, or interaction probability, of capture by a flux Φ of incoming particles, and N represents a number density of isotope *i* or *i*-1. Number densities are calculated as follows:

$$N = \frac{\rho N_{Av}}{MM} \tag{30}$$

where ρ is the density, N_{Av} is Avogadro's number, and MM is the molar mass (or molecular weight). Note that the macroscopic cross section Σ accounts for both the amount of isotope *i*-1 present and the probability that isotope *i*-1 undergoes a reaction to produce isotope *i*:

$$\Sigma = N\sigma \tag{31}$$

6.2 Setting Up a Physical Model

These can be constructed into a series of differential equations, which can be solved to obtain the concentrations of different isotopes. For example, let's say we have a quantity of isotope N₁ at N₁₀, and it decays into isotope N₂, which also decays into isotope N₃. Isotope N₂, however, also captures neutrons (that's right, we're in a reactor now) with a characteristic cross section σ_{c_2} :

$$\frac{dN_1}{dt} = -\lambda_1 N_1 \tag{32}$$

$$\frac{dN_2}{dt} = \lambda_1 N_1 - \lambda_2 N_2 - N_2 \sigma_{c_2} \Phi_{reactor}$$
(33)

$$\frac{dN_3}{dt} = \lambda_2 N_2 \tag{34}$$

Things to keep in mind include:

- 1. Cases in which coefficients are wildly different, for example, what happens if $\lambda_1 \gg \lambda_2$ or $\lambda_1 \ll \lambda_2$?
- 2. Behavior during very short times
- 3. Finding maximum concentrations of a given isotope, by setting the derivative equal to zero

6.3 An Example Full Derivation

Let's say we have the following nuclear reactions (like on the lecture on October 6th), where we are producing ⁶⁰Co from the neutron bombardment of ⁵⁹Co, and ⁶⁰Co has its own decay constant λ where it decays by β^- decay into ⁶⁰Ni:

$$\underbrace{\overset{59}{_{27}Co}}_{N_1} \xrightarrow{n} \underbrace{\overset{60}{_{27}Co}}_{N_2} \xrightarrow{\lambda} \underbrace{\overset{60}{_{28}Ni}}_{N_3} Ni \tag{35}$$

We also have to account for the fact that both 59 Co and 60 Co are "burned" in the reactor by capturing neutrons. The first reaction produces 60 Co, while the second one depletes it. We therefore define a couple of *neutron capture cross sections*:

$$\sigma_{c_{59C_{2}}} = \sigma_{59} = 20 \, b \qquad \sigma_{c_{560}} = \sigma_{60} = 2 \, b \qquad 1 \, b = 10^{-24} \, cm^2 \tag{36}$$

where we have looked up the values of the cross sections from the JANIS database, using the ENDF VII library for incident neutron data, and we've chosen the values at 0.025eV (the kinetic energy of thermal neutrons). Let's just pretend that our reactor has only thermal neutrons in it, a "one group" approximation. Oh, let's also define the neutron flux of our reactor, or the number of neutrons zipping through every square centimeter per second:

$$\Phi = 10^{14} \frac{n}{cm^2 s} \tag{37}$$

We next look up the half life of 60 Co, and use Equation 27 to get its decay constant:

$$t_{1/2} = 1925.4 \, days = 1.66 \cdot 10^8 s \qquad \lambda = \frac{\ln(2)}{1.66 \cdot 10^8 s} = 4.17 \cdot 10^{-9} s^{-1} \tag{38}$$

Finally, we have to define some initial amount of 59 Co that we put into our reactor. Let's just say it was 100g of 59 Co, or 1.69 moles, or 10^{24} atoms:

$$N_{10} = 10^{24} atoms \tag{39}$$

Finally we are ready to construct our differential equations to physically model this real system. First, we recognize from the KAERI Table of Nuclides that ⁵⁹Co is stable, so it has no production term, and the only way for it to be destroyed is to be "burned" by neutron capture:

$$\frac{dN_1}{dt} = -\sigma_{59}\Phi N_1 \tag{40}$$

Next, the production rate of 60 Co is equal to the destruction rate of 59 Co, while 60 Co can be destroyed both by natural radioactive decay and artificial "burning:"

$$\frac{dN_2}{dt} = \sigma_{59}\Phi N_1 - \sigma_{60}\Phi N_2 - \lambda N_2 \qquad \frac{dN_2}{dt} = \sigma_{59}\Phi N_1 - (\lambda + \sigma_{60}\Phi)N_2 \tag{41}$$

Finally, the only way to produce 60 Ni is by radioactive decay of 60 Co. Note that "burning" 60 Co does NOT produce 60 Ni:

$$\frac{dN_3}{dt} = \sigma_{60} \Phi N_2 \tag{42}$$

Here we are ignoring the "burning" of 60 Ni. In fact, let's just ignore 60 Ni altogether, because we don't care about it:

$$\frac{dN_3}{dt} = \sigma_{60} \Phi N_2 \tag{43}$$

Now we start with the easy equation for N_1 (t). Note that the quantity $\sigma_{59}\Phi$ has the same units as λ , so the equation takes the same form:

$$\frac{dN_1}{dt} = (-\sigma_{59}\Phi)N_1 \qquad \int \left(\frac{dN_1}{N_1}\right) = \int (-\sigma_{59}\Phi)dt \qquad N_1(t=0) = N_{10} \qquad N_1(t) = N_{10}e^{-\sigma_{59}\Phi t}$$
(44)

Now we take this expression for N_1 and substitute it into Equation 41:

$$\frac{dN_2}{dt} = \sigma_{59} \Phi N_{10} e^{-\sigma_{59} \Phi t} - (\lambda + \sigma_{60} \Phi) N_2$$
(45)

Next we rearrange terms so that all the stuff is on one side of the equation:

$$\frac{dN_2}{dt} + (\lambda + \sigma_{60}\Phi) N_2 - \sigma_{59}\Phi N_{10}e^{-\sigma_{59}\Phi t} = 0$$
(46)

Next we introduce our *integrating factor*, μ :

$$\mu = e^{\int (\lambda + \sigma_{60}\Phi)dt} = e^{(\lambda + \sigma_{60}\Phi)t} \tag{47}$$

and we multiply every term in Equation 46 by μ :

$$\left(\frac{dN_2}{dt}\right)e^{(\lambda+\sigma_{60}\Phi)t} + \left(\left(\lambda+\sigma_{60}\Phi\right)N_2\right)e^{(\lambda+\sigma_{60}\Phi)t} - \left(\sigma_{59}\Phi N_{10}e^{-\sigma_{59}\Phi t}\right)e^{(\lambda+\sigma_{60}\Phi)t} =$$
(48)

We recognize that our first two terms look eerily similar to the end result of the Product Rule:

$$\frac{d\left(a\left(t\right)b\left(t\right)\right)}{dt} = a\left(t\right)\frac{db\left(t\right)}{dt} + \frac{da\left(t\right)}{dt}b\left(t\right) \qquad equivalently \qquad (ab)' = ab' + a'b \tag{49}$$

We then smoosh the first two terms of Equation 48 together using the Product Rule in reverse, and combine the exponential parts of the third term:

$$\frac{d\left(N_2 e^{(\lambda+\sigma_{60}\Phi)t}\right)}{dt} = \sigma_{59}\Phi N_{10}e^{((\lambda+\sigma_{60}\Phi)-\sigma_{59}\Phi)t}$$
(50)

We then integrate both sides:

$$\int \left(\frac{d\left(N_2 e^{(\lambda+\sigma_{60}\Phi)t}\right)}{dt}\right) dt = \int \left(\sigma_{59}\Phi N_{10} e^{((\lambda+\sigma_{60}\Phi)-\sigma_{59}\Phi)t}\right) dt$$
(51)

This just kills the derivative on the left hand side, puts the exponential term in the denominator on the right hand side, and introduces a constant of integration:

$$N_2 e^{(\lambda + \sigma_{60}\Phi)t} = \frac{\sigma_{59}\Phi N_{10}}{((\lambda + \sigma_{60}\Phi) - \sigma_{59}\Phi)} e^{((\lambda + \sigma_{60}\Phi) - \sigma_{59}\Phi)t} + C$$
(52)

We now use the initial condition that we had no 60 Co when we first started producing it at t = 0:

$$N_{2}(t=0) = 0 \qquad \mathcal{N}_{2}e^{(\lambda+\sigma_{60}\Phi)t} = \frac{\sigma_{59}\Phi N_{10}}{((\lambda+\sigma_{60}\Phi)-\sigma_{59}\Phi)}e^{((\lambda+\sigma_{60}\Phi)-\sigma_{59}\Phi)t} + C$$
(53)

$$\underbrace{(0) e^{(\lambda + \sigma_{60}\Phi)(1)}}_{(0)} = \frac{\sigma_{59}\Phi N_{10}}{((\lambda + \sigma_{60}\Phi) - \sigma_{59}\Phi)} \underbrace{e^{((\lambda + \sigma_{60}\Phi) - \sigma_{59}\Phi)(0)}}_{(0)} + C$$
(54)

$$0 = \frac{\sigma_{59}\Phi N_{10}}{((\lambda + \sigma_{60}\Phi) - \sigma_{59}\Phi)} + C \qquad C = \frac{-\sigma_{59}\Phi N_{10}}{((\lambda + \sigma_{60}\Phi) - \sigma_{59}\Phi)}$$
(55)

We finally plug this integration constant back into Equation 52 and do a bit of rearranging:

$$N_2 e^{(\lambda + \sigma_{60}\Phi)t} = \frac{\sigma_{59}\Phi N_{10}}{((\lambda + \sigma_{60}\Phi) - \sigma_{59}\Phi)} e^{((\lambda + \sigma_{60}\Phi) - \sigma_{59}\Phi)t} - \frac{\sigma_{59}\Phi N_{10}}{((\lambda + \sigma_{60}\Phi) - \sigma_{59}\Phi)}$$
(56)

$$N_2 e^{(\lambda + \sigma_{60}\Phi)t} = \frac{\sigma_{59}\Phi N_{10}}{((\lambda + \sigma_{60}\Phi) - \sigma_{59}\Phi)} \left[e^{((\lambda + \sigma_{60}\Phi) - \sigma_{59}\Phi)t} - 1 \right]$$
(57)

$$\frac{N_{2}e^{(\lambda\pm\sigma_{60}\Phi)t}}{e^{(\lambda\pm\sigma_{60}\Phi)t}} = \frac{\sigma_{59}\Phi N_{10}}{((\lambda+\sigma_{60}\Phi)-\sigma_{59}\Phi)} \left[\frac{e^{((\lambda\pm\sigma_{60}\Phi)-\sigma_{59}\Phi)t}}{e^{(\lambda\pm\sigma_{60}\Phi)t}} - \frac{1}{e^{(\lambda+\sigma_{60}\Phi)t}}\right]$$
(58)

$$N_{2}(t) = \frac{\sigma_{59} \Phi N_{10}}{\left((\lambda + \sigma_{60} \Phi) - \sigma_{59} \Phi \right)} \left[e^{(-\sigma_{59} \Phi)t} - \frac{1}{e^{(\lambda + \sigma_{60} \Phi)t}} \right]$$
(59)

$$N_2(t) = \frac{\sigma_{59} \Phi N_{10}}{((\lambda + \sigma_{60} \Phi) - \sigma_{59} \Phi)} \left[e^{-(\sigma_{59} \Phi)t} - e^{-(\lambda + \sigma_{60} \Phi)t} \right]$$
(60)

Not surprisingly, this looks *exactly* like Equation 4.40 from the Turner book:

$$N_2(t) = \frac{\lambda_1 N_{10}}{(\lambda_2 - \lambda_1)} \left[e^{-\lambda_1 t} - e^{-\lambda_2 t} \right]$$
(61)

where we have defined $\lambda_1 = \sigma_{59} \Phi$ and $\lambda_2 = \lambda + \sigma_{60} \Phi$. Now let's start plugging in some of the values:

$$\lambda_1 = \sigma_{59} \Phi = \left(20 \cdot 10^{-24} \, \text{cm}^2\right) \left(10^{14} \frac{n}{\text{cm}^2 s}\right) = 2 \cdot 10^{-9} s^{-1} \tag{62}$$

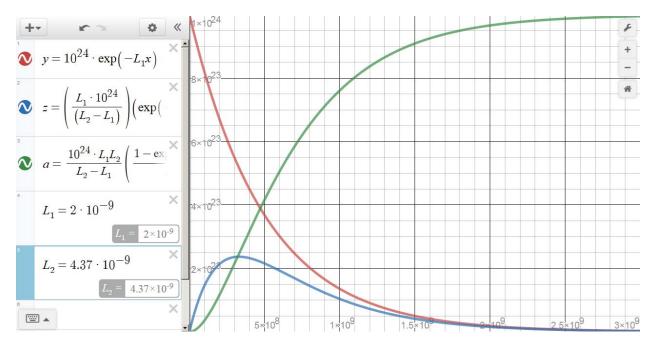
$$\lambda_2 = \lambda + \sigma_{60}\Phi = \left(4.17 \cdot 10^{-9} \frac{1}{s}\right) + \left(2 \cdot 10^{-24} \text{cm}^2\right) \left(10^{14} \frac{n}{\text{cm}^2 s}\right) = 4.37 \cdot 10^{-9} s^{-1} \tag{63}$$

How we plug these values into Equation 61:

$$N_{2}(t) = \frac{\left(2 \cdot 10^{-9} s^{-t}\right) \left(10^{24} a toms\right)}{\left(4.37 \cdot 10^{-9} s^{-t} - 2 \cdot 10^{-9} s^{-t}\right)} \left[e^{-\left(2 \cdot 10^{-9} s^{-1}\right)t} - e^{-\left(4.37 \cdot 10^{-9} s^{-1}\right)t}\right]$$
(64)

$$N_2(t) = \frac{\left(2 \cdot 10^{15} a toms\right)}{\left(2.37 \cdot 10^{-9} s^{-1}\right)} \left[e^{-\left(2 \cdot 10^{-9} s^{-1}\right)t} - e^{-\left(4.37 \cdot 10^{-9} s^{-1}\right)t} \right]$$
(65)

We can then graph this situation using Desmos:



Note that the x-axis is in seconds, and the y-axis is in atoms. This shows you that it takes about $3 \cdot 10^8$ seconds, or 10 years, to reach a maximum inventory of 60 Co in the reactor. A very real example, using actual numbers, from a very theoretical derivation!

22.01 Introduction to Nuclear Engineering and Ionizing Radiation Fall 2016

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