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MC312, Modeling and Simulation

In the following lab, we have discussed the numerical and analytical methods of solving the problem of Radioactive Chain Decay. We study a particular scenario that includes one radioactive object decaying into another radioactive object, creating a chain of such objects. Our key findings pertaining to the maximum total disintegration of the radioactive substance provided the conditions given in transient and secular equilibrium.

I. INTRODUCTION

The phenomenon of radioactive decay can be comprehensively explained through the usage of compartmental models and concisely represented as ordinary differential equations. The decay process of a radioactive substance involves the degradation of its mass in direct proportion to its remaining mass. In the context of this report, our scope extends to investigating the intricate dynamics of radioactive decay within a sequential chain of elements. In our chain decay scenario, the process unfolds through a sequence of disintegrations involving multiple distinct elements. Substance A undergoes decay to transform into substance B, subsequently leading to the decay of substance B into a new element, C. The rates of disintegration for each radioactive element are inherently linked to their individual masses and unique decay constants. The compartmental model emerges as a tool to comprehend this complex decay chain. By encapsulating all three elements within a single compartment, we can systematically analyze the interplay between inflow and outflow.

II. MODEL

Considering only a single radioactive substance, the rate of decay will be directly proportional to the mass of that substance. Therefore, the mathematical expression for such a substance A can be written as:

$$\frac{dA}{dt} = -aA\tag{1}$$

In the above equation a is the decay rate constant.

Our main focus of discussion is on the problem where we will be dealing with 3 different substances with different decay constants. This is a case where A disintegrates into B and B disintegrates into C. Since the decay rate depends on the masses of the substances we can confidently consider A, B, and C to be modeled separately meaning for A, as mentioned previously its mass is proportional to its decay rate. For B, its mass will always be equal to the mass gained via the

disintegration of substance A minus the mass lost via its own disintegration into substance C. For substance C, the rate at which it will gain mass will be equal to the mass lost from substance B. Coming to the mathematical model for this problem. Given that a and b are the decay constants of substance A and B respectively we have:

$$\frac{dA}{dt} = -aA\tag{2}$$

$$\frac{dB}{dt} = aA - bB \tag{3}$$

$$\frac{dC}{dt} = bB \tag{4}$$

Assumptions to be made are, A_0 is considered to be the initial mass of substance A, while the initial masses of B and C are to be presumed 0.

III. RESULTS

Fig. 1 shows the normal and typical behavior of the radioactive substances when put in the scenario mentioned previously. We have assumed the decay constants a and b to be a = $0.2 \, \mathrm{s}^{-1}$ and b = $0.3 \, \mathrm{s}^{-1}$ respectively. The initial mass of substance A is 10g and that of B and C is assumed to be 0.

Our observations reveal a distinct pattern in the behavior of element A, exhibiting a clear exponential decrease over time. Element A experiences continuous disintegration at a constant rate denoted by a unaided by any influx from other radioactive sources. Consequently, the mass of A diminishes steadily as time progresses. This decline aligns with the analytical solution derived from equation 2, reinforcing the anticipation of exponential decay in element A.

In contrast, the trajectory of substance B unfolds differently. Initially, its mass experiences a rapid increase, reaching a peak before embarking on a gradual

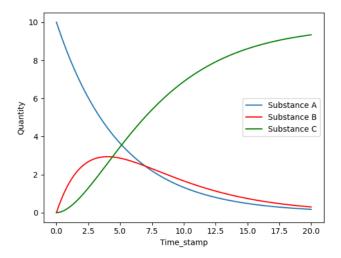


FIG. 1: Decay Rate of the 3 chains of substances over time

decline. Substance B emerges as a direct result of the radioactive decay process occurring in substance A. During the initial stages, the mass of B remains negligible, leading to a correspondingly low disintegration rate—proportional to its small mass—and a decay constant b significantly smaller than a As a consequence, the inflow of mass from A to B outweighs the outflow, causing an accumulation of substance B. However, as time elapses, the inflow from A diminishes exponentially while the outflow from B remains constant, ultimately resulting in a decline in the net quantity of B.

Meanwhile, substance C displays a distinct trend characterized by rapid growth. As the mass of substance B expands, its inherent radioactivity also intensifies, contributing to the exponential increase in substance C. The growth rate of C remains intrinsically tied to the quantity of substance B throughout this progression. After a certain duration, the rate of C's increase gradually subsides, transitioning to a linear pattern. Notably, the graph depicting substance C approaches an asymptote represented by the value A_0 , indicating a convergence towards a specific limit.

A. Maximum Total Radioactivity

Fig. 2 shows the total radioactive activity of the substances where we have taken the value of b to be constant $b = 0.3 \text{ s}^{-1}$ and various values of a.

We have basically plotted different maximum total radioactivity values for a constant value of b while we vary to value of a from 0.1 to 1. We calculate the total radioactivity by the equation:

$$TR = aA + bB \tag{5}$$

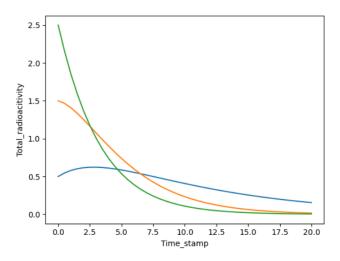


FIG. 2: Change in Radioactivity with different values of a

where TR is the 'Total Radioactivity'. From the plot of our graph, we notice that the peak shifts towards the left as the parameter a experiences an increment. The rate of decay for substance A is intrinsically linked to the value of a: smaller a values correspond to diminished disintegration rates, while larger a values entail accelerated decay. Meanwhile, for a constant b, the disintegration rate of substance B hinges upon its own mass, denoted as B.

When a is smaller than b, an intriguing pattern emerges. Initially, a lesser amount of substance A decomposes into B, leading to a small inflow of mass into B. Consequently, B's disintegration rate is proportionally modest due to this initial influx. However, B possesses a higher decay constant, prompting a significant portion of its mass to decay as soon as it is transferred from A. In this scenario, the overall radioactivity is lower due to the comparatively smaller decay constant a and the constant low mass of B. Gradually, as the mass of B increases, the number of disintegrations intensifies, causing the total radioactivity to experience a slow rise, culminating in a peak value.

Conversely, when a surpasses b, a distinct behavior arises. The initial decay rate of A is maximized, resulting in the highest number of atom decays during the initial phase. Similarly, substance B exhibits an elevated inflow initially, leading to a correspondingly high disintegration rate. As a consequence, the peak of the total radioactivity graph is elevated and positioned closer to the origin.

In essence, the intricate interplay between a and b governs the dynamics of total radioactivity, with their relative values shaping the temporal evolution and characteristics of the radioactivity curve. The changes in C are governed by B.

B. Transient Equilibrium

To come up with differential equations that include the maximum amount of substance B and the time at which this takes place, we have to go back to the first 3 equations that were discussed in this report.

$$\frac{dA}{dt} = -aA$$

$$\frac{dA}{A} = -adt$$

$$\int_{A_0}^{A} \frac{1}{A} dA = \int_{0}^{t} adt$$

$$\ln \frac{A}{A_0} = -at$$

Hence, we deduce the following equation:

$$A = A_0 e^{-at} \tag{6}$$

Now we are already given the equation in the prompt:

$$B = \frac{aA_0}{b-a} \left(e^{-at} - e^{-bt} \right) \tag{7}$$

Eq. 7 can be verified using Eq. 6 as below:

$$\frac{dB}{dt} = \left(\frac{aA_0}{b-a}\right) \frac{d}{dt} \left(e^{-at} - e^{-bt}\right)$$

$$\frac{dB}{dt} = \left(\frac{aA_0}{b-a}\right) \left[\left(-ae^{-at} + be^{-bt}\right) + \left(be^{-at} - be^{-at}\right)\right]$$

$$\frac{dB}{dt} = \left(\frac{aA_0}{b-a}\right) \left[(b-a)e^{-at} + b\left(e^{-bt} - e^{-at}\right)\right]$$

$$\therefore \frac{dB}{dt} = \frac{dA}{dt} - bB$$

Now taking into account that a < b, we notice that the term e^{-bt} tends to 0 and hence it can be neglected. Therefore, we are left with:

$$B = \frac{aA_0}{b-a} \left(e^{-at} \right) \tag{8}$$

Substituting the value of A from Eq. 6 in Eq. 8:

$$\frac{B}{A} \approx \frac{a}{b-a} \tag{9}$$

For a > b, we notice that the graph given below is diverging since it implies that the decay rate of the substance corresponding to a is faster than that of the substance corresponding to b. In this scenario, the substance with the faster decay rate will approach equilibrium more quickly, and its concentration will continue to increase. Since the slower decaying substance's production rate can't keep up with the faster decay, its concentration will keep decreasing. This leads to a divergence in the

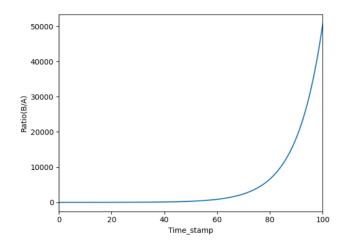


FIG. 3: Ratio of A/B vs Time for a > b

graph as the concentrations of the two substances move in opposite directions over time.

To prove the above analytically we refer to Eq. 7. We further solve this equation by putting in the value of A from Eq 6. as:

$$\frac{B}{A} = \frac{a}{b-a} \left(1 - \frac{e^{at}}{e^{bt}} \right)$$
$$\frac{B}{A} = \frac{a}{a-b} \left(\frac{e^{at} - e^{bt}}{e^{bt}} \right)$$

Since a > b, e^{at} > e^{bt} and therefore, the e^{bt} in the numerator can be exempted. On solving, we arrive at:

$$\frac{B}{A} = \frac{a}{a-b} \left(e^{(a-b)t} \right) \tag{10}$$

C. Maximum mass of second substance in the given Scenario

From Eq. 7 we can directly calculate the amount of substance B at any given time. To deduce the maximum amount we just have to differentiate that equation which goes as follows:

$$\frac{dB}{dt} = \left(\frac{aA_0}{b-a}\right)\frac{d}{dt}\left(e^{-at} - e^{-bt}\right)$$

and take $\frac{dB}{dt} = 0$. Hence,

$$e^{(a-b)t_{\max}} = \frac{a}{b}$$
$$\therefore t_{\max} = \frac{\ln(a) - \ln(b)}{a - b}$$

Using this, we get,

$$B_{\text{max}} = \left(\frac{aA_0}{b-a}\right) \left[\left(\frac{a}{b}\right)^{\frac{a}{b-a}} - \left(\frac{a}{b}\right)^{\frac{b}{b-a}} \right]$$

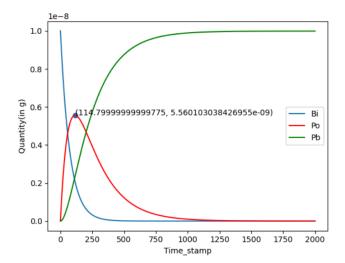


FIG. 4: Maximum mass of Polonium-210

To put this pictorially, we consider the example where Bismuth-210 decays into Polonium-210 whch in turn decays into Lead-206 with decay constant of $Bi^{210} = 0.0137/da$ and decay constant of $Po^{210} = 0.0051/da$ and initial amount of $Bi^{210} = 10^{-8}$ gms. The above graph inculcates the time and the amount at which we notice

the maximum value of Polonium-210.

IV. CONCLUSIONS

In summary, we've explored a basic mathematical framework representing the decay of radioactive elements within a sequential chain. This approach, known as the compartment model, proves to be an effective method for simulating interconnected radioactive elements. Through our mathematical model, we're able to make precise predictions and observations about these elements' characteristics. This approach proves particularly useful in scenarios where decay rates vary across different stages or elements. Moreover, we delve into the connections among the decay rates, highlighting the prerequisites for the emergence of both transient and secular equilibrium states. To wrap up, we compute the utmost mass achievable by the central element, along with the corresponding timing of this maximum, all in terms of the decay rates denoted as a and b. Overall this lab has taught us the process of conducting numerical experiments and comparing them to analytical solutions to have a concrete foundation on the process and the workings of the compartment model.