

Lab - 1

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CS-302, Modeling and Simulation*

In this lab we numerically and analytically analyze the radioactive chains of length three. We will also look into various type of equilibrium which are exhibited by radioactive chains of length 3. We will also analyze how amount of radioactive substance behaves with time and when maximum total radioactivity occurs.

INTRODUCTION

Radioactivity is the process by which an unstable atomic nucleus loses energy by radiation. Radioactive chains refers to a series of radioactive decays of different radioactive products in a series of transformations. For a radioactive element, rate of decay is directly proportional to its mass, i.e.,

$$\frac{dN}{dt} = -\lambda N$$

here λ is decay constant of radioactive element.

MODEL

If a radioactive substance, substance A, decays into substance substance B, we say that substance A is the parent of substance B and that substance B is the child of substance A. If substance B is also radioactive, substance B is the parent of another substance, substance C, and we have a chain of substances. Here we will assume that substance C is not radioactive so that chain stops at substance C.

We know that the rate of disintegration of a radioactive substance at any time is equal to disintegration constant for that substance multiplied by amount of substance present at that time. We will assume that no any other interaction happens between substances other than disintegration and no substance is added from outside. So, rate of change for any substance is equal to inflow (i.e., disintegration of parent nuclei) minus outflow (i.e., it's own disintegration) of that substance.

$$\frac{dA(t)}{dt} = -aA(t) \quad (1)$$

$$\frac{dB(t)}{dt} = aA(t) - bB(t) \quad (2)$$

$$\frac{dC}{dt} = bB(t) \quad (3)$$

A, B and C are amounts of substance A, substance B and substance C respectively.

a and b disintegration constant of substance A and substance B respectively.

Solving Eq. (1), (2) and (3) we get,

$$A(t) = A_0 e^{-at} \quad (4)$$

$$B(t) = \frac{a}{b-a} A_0 (e^{-at} - e^{-bt}) + B_0 e^{-bt} \quad (5)$$

$$C(t) = A_0 \left(1 - \frac{b}{b-a} e^{-at} + \frac{a}{b-a} e^{-bt}\right) - B_0 e^{-bt} \quad (6)$$

From here on we will consider that initial amount of substance B and substance C is zero, whereas initial amount of substance A was A_0 .

RESULTS

Plots and Observations

Fig. 1 shows how amount of A, B and C changes with time. Here, amount of A decreases exponentially with time. As the rate of change of A is negatively proportional to the amount of substance A, decrease in the amount of A will increase its rate (but will never make it positive). Thus, A decreases with increasing (lesser negative) rate. Also, amount of C is found to be increasing with time, it is true as substance C doesn't disintegrate but substance B disintegrates into substance C. Also, once amount of substance B starts decreasing, amount of substance C will still grow but with a decreasing rate. Amount of substance B will increase until A decays more as compared to B (i.e., $aA > bB$) and after it happens B will decay more than A and its mass will reduce thereafter.

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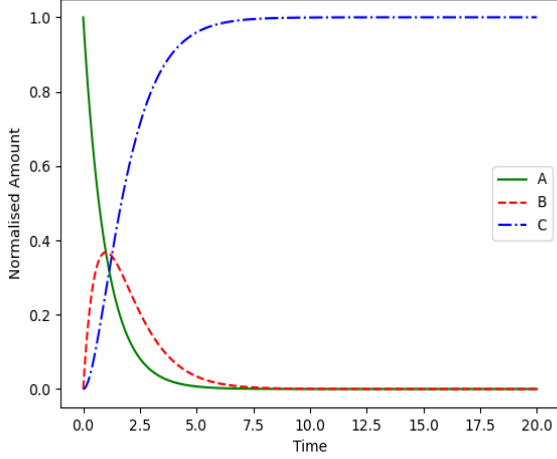


Fig. 1: Plots of Normalized Amount of Substances A, B, C v/s Time. Values of a , b and A_0 was set 1, 1 and 10 respectively.

Maxima of Substance B

First of all, let's get equation for time at which amount of B will get its maximum value. Taking differentiation of Equation (5) on both side we get,

$$\frac{dB}{dt} = \frac{a}{b-a} A_0 (-ae^{-at} + be^{-bt}) \quad (7)$$

Substituting $\frac{dB}{dt} = 0$, we get

$$t_m = \frac{1}{b-a} \ln\left(\frac{b}{a}\right) \quad (8)$$

We can see that t_m depends only on values of a and b . Also, for both the cases of $a < b$ and $b < a$, t_m will be positive. So, we can say that curve of B will have one maxima or one minima. Now, we must find sets of values of a and b for which we will get maxima and set of values of a and b for which we will get minima.

Taking differentiation on both side of equation (7), we get,

$$\frac{d^2B}{dt^2} = \frac{a}{b-a} A_0 (a^2 - b^2 e^{(a-b)t}) \quad (9)$$

Substituting $t = t_m$, equation (9) becomes,

$$\left(\frac{d^2B}{dt^2}\right)_{t=t_m} = \frac{a}{b-a} A_0 (a^2 - b^2 \left(\frac{a}{b}\right)) = -a^2 A_0 \quad (10)$$

As $a > 0$ and $A_0 > 0$, value of $\frac{d^2B}{dt^2}$ will be less than zero for all set of values of a and b . Thus, curve of B will always have a maxima at time t_m .

Types of Equilibrium

1. Secular Equilibrium

If in some radioactive chain of length three, amount of substance A and substance B tends to become constant as t tends to infinity then that radioactive chain is said to be acquiring secular equilibrium. Secular equilibrium occurs when $a \ll b$. Lets try to get value of amount of A and B as t tends to infinity.

From equation (5), putting $B_0 = 0$ we get,

$$B = \frac{a}{b-a} A_0 e^{-at} (1 - e^{(a-b)t}) \quad (11)$$

As $t \rightarrow \infty$, $e^{(a-b)t} \rightarrow 0$ as $a - b < 0$, so equation 11 becomes,

$$B = \frac{a}{b-a} A_0 e^{-at} \quad (12)$$

As a is very small we can assume $e^{-at} \approx 1$ for a sufficiently small value of t , thus equation (12) becomes,

$$B = \frac{a}{b-a} A_0 \quad (13)$$

Using equation (4) and assuming $e^{-at} \approx 1$ for a sufficiently small value of t , we get,

$$A = A_0 \quad (14)$$

Moreover, lets compare rate of disintegration of A (equals to aA) and B (equals to bB) as t tends to infinity,

$$\frac{aA}{bB} = \frac{b-a}{a} * \frac{a}{b} \quad (15)$$

As $a \ll b$,

$$\frac{aA}{bB} = 1 - \frac{a}{b} \approx 1 \quad (16)$$

Secular Equilibrium is observed in radioactive chain of radium-226 to radon-222 to polonium-218 ($\text{Ra}^{226} \rightarrow \text{Rn}^{222} \rightarrow \text{Po}^{218}$). Here, value of a is 0.00000117/da and value of b is 0.181/da.

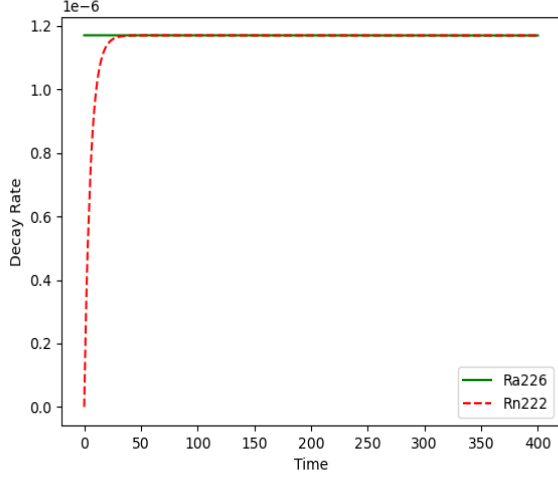


Fig. 2: Decay Rate of A and B v/s Time

In Fig. 2, we can observe that decay rate of Ra-226 and Rn-222 becomes equal after certain time (as $a \ll b$). Moreover, the time at which this will happen is t_m from equation (8).

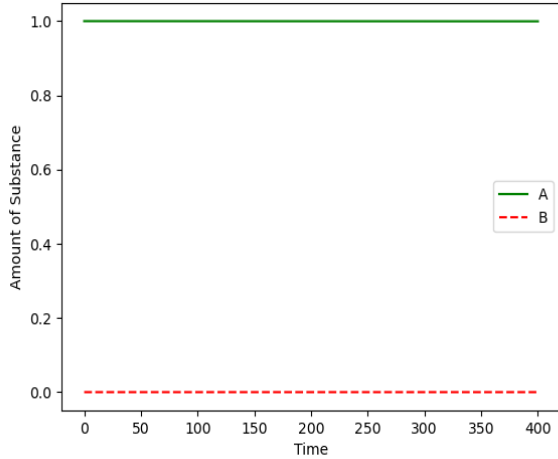


Fig. 3: Amount of Substance v/s Time

Observe in Fig. 3 that Amount of substance Ra-226 and Rn-222 remains almost same. But, if we consider plots for very large t , amount of Ra-226 will decrease and Rn-222 increases up-to time t_m and then decreases.

2. Transient Equilibrium

Transient Equilibrium is said to occur when the parent nuclei has decay constant smaller as compared to the parent nuclei i.e., $a < b$. We can show that ratio of $\frac{B}{A}$ becomes constant as t tends to infinity. Lets consider equation (11) and as $a < b$, $e^{(a-b)t} \rightarrow 0$ as $t \rightarrow \infty$ and thus we are left with,

$$B = \frac{a}{b-a} A_0 e^{-at} \quad (17)$$

Using Equation (17) and (4) we get,

$$\frac{B}{A} = \frac{a}{b-a} \quad (18)$$

Note that A tends to 0 as t tends to infinity and so does B from equation (17).

Transient Equilibrium may look similar to that of secular equilibrium but it is quite different. In transient equilibrium ratio of amount of substance A and B becomes constant however in secular equilibrium amount of substance A and B itself becomes constant. Another difference is that, in secular equilibrium, ratio decay rate of A and B tends to 1 as t tends to infinity, whereas this ratio is smaller than 1 for transient equilibrium.

3. No Equilibrium

No Equilibrium occurs when the decay rate of parent nuclei is larger compared to the decay rate of daughter nuclei i.e., $a > b$.

Multiplying and dividing $e^{(a-b)t}$ on right side of equation (11), we get,

$$B = \frac{a}{b-a} A_0 e^{-bt} (e^{(b-a)t} - 1) \quad (19)$$

As $a > b$, $e^{(b-a)t} \rightarrow 0$ as $t \rightarrow \infty$ and thus we are left with,

$$B = \frac{a}{a-b} A_0 e^{-bt} \quad (20)$$

Dividing A on both side of equation (20) we get,

$$\frac{B}{A} = \frac{a}{a-b} e^{(a-b)t} \quad (21)$$

We can see that $e^{(a-b)t} \rightarrow \infty$ as $t \rightarrow \infty$ and so will $\frac{B}{A}$. Thus, we can say that ratio of $\frac{B}{A}$ don't approach a number as $t \rightarrow \infty$. We can see such Equilibrium in radioactive chain $\text{Bi}^{210} \rightarrow \text{Po}^{210} \rightarrow \text{Pb}^{206}$, where $a = 0.0137/\text{da}$ and $b = 0.0051/\text{da}$. (refer Fig. 4 for $\frac{B}{A}$ vs t plot)

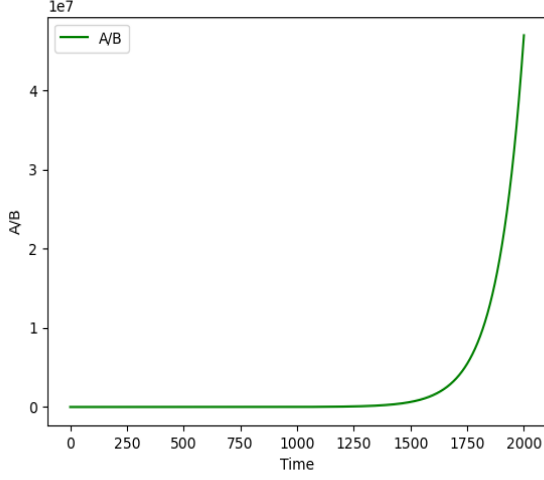


Fig. 4 : Ratio of amount of Bi^{210} to amount of Po^{210} v/s Time

Maximum Total Radioactivity

Total Radioactivity(T) at any time t is total amount of decay that occurred at time t . So total radioactivity at time t equals to $aA + bB$. Now, if we differentiate $aA + bB$ and make it equal to zero then we get,

$$t_{rm} = \frac{1}{b-a} \ln\left(\frac{b^2}{2ab - a^2}\right) \quad (22)$$

Here, let's show that logarithm is always greater than 1 as,

$$\frac{b^2}{2ab - a^2} = \frac{1}{2\frac{a}{b} - \frac{a^2}{b^2}} \quad (23)$$

Now, let's assume $2\frac{a}{b} - \frac{a^2}{b^2} < 1$, so,

$$\begin{aligned} 2\frac{a}{b} &< 1 + \frac{a^2}{b^2} \\ 2 &< \frac{a}{b} + \frac{b}{a} \\ 2ab &< a^2 + b^2 \\ 0 &< a^2 - 2ab + b^2 \\ 0 &< (a - b)^2 \end{aligned}$$

So, if our assumption was right and thus term inside logarithm in equation (22) is always greater than 1 and so value of logarithm is always positive.

Thus, if $a < b$, then t_{rm} is positive and thus a maxima will exist in curve of T. On the other hand, if $a > b$, then t_{rm} is negative and so no maximum value will occur at $t = 0$ and thereon it will decrease (observe this in Fig. 5).

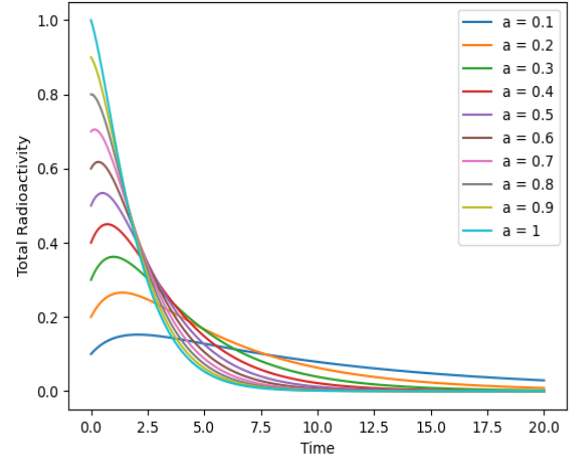


Fig. 5: Total Radioactivity for various values of a and $b = 0.8$ v/s Time

Conclusion

Double Compartmental Model proves to be an important tool for modelling & analysing of the Radioactive Chains. In this lab, we observed how mass of each radioactive element changes in chain of length 3. We also learned about various types of equilibrium and conditions under which they occur. We analysed maxima of substance B (middle element in the chain) and maxima of total radioactivity and how values of decay constants affect it.