

Lab -1

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 CS302, Modeling and Simulation*

In this lab we numerically and analytically analyze the three element chain reactions of radioactivity for different values of disintegration constants of each of them. Our main observations are that the values of the disintegration constants affect the state of equilibrium achieved and the total radioactivity of a given decay chain.

I. INTRODUCTION

Radioactive decay of an element can be modeled as a differential equation. If $Q(t)$ is the mass of the substance then it decays at a rate, r , which is known as the disintegration constant. The differential equations used in this problem are modeled as follows. [1].

II. MODEL

We have a three element radioactive chain. Let the three elements be A, B and C. We assume that the disintegration constant of A is a and that of B is b . Then, the mass of A that disintegrates into B in unit time is aA . The mass of B that disintegrates into C in unit time is bB . This can be modeled using the following differential equations.

$$\dot{A} = -aA \quad (1)$$

$$\dot{B} = aA - bB \quad (2)$$

$$\dot{C} = bB \quad (3)$$

Eq. (1) is the differential equation for the radioactive decay of element A, that is, it represents the change in mass of A as time progresses. Eq. (2) is the differential equation for the radioactive decay of element B and it represents the change in mass of B as time progresses. The same follows with Eq. (3), it represents the same for element C. The solutions to the differential equations are as follows:

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

$$B = \frac{aA_0(e^{-at} - e^{-bt})}{b - a} \quad (5)$$

III. RESULTS

(a)

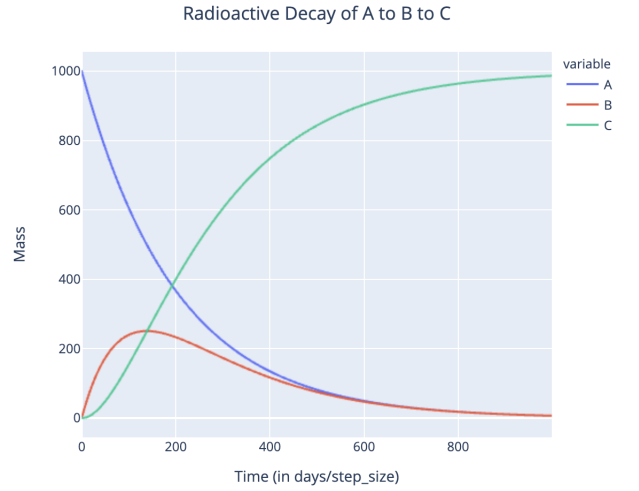


FIG. 1. Three element radioactive chain. Here, $a = 0.5$ and $b = 1$.

(b) In the figure above, disintegration constant of A is 0.5 and that of B is 1. We can see that as time progresses, A disintegrates and hence its mass decreases. On the other hand, as A disintegrates into B, initially, the mass of B starts increasing, until a point where B itself starts disintegrating, and hence its mass also starts decreasing. Meanwhile, as B begins to disintegrate, mass of C starts increasing and after a point, when A and B have almost completely disintegrated into C, we see that the mass of C is almost equal to the initial mass of A.

(c) From Fig. (2), we can see that as a goes from 0.1 to 1, the time of maximum total radioactivity decreases. This is because as a increases, the disintegration happens faster and hence, the peak of total radioactivity is achieved faster.

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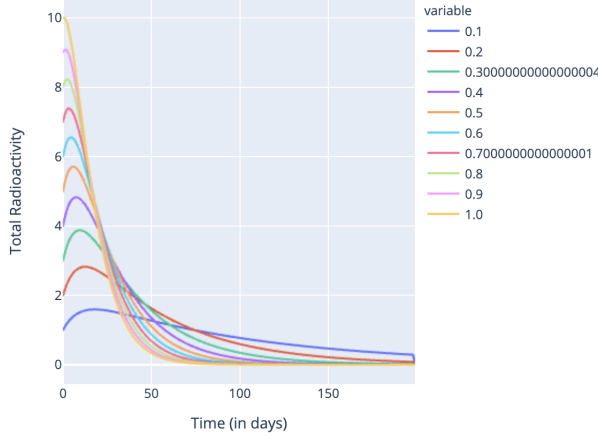


FIG. 2. Total radioactivity w.r.t. time as the disintegrating factor increases.

The total radioactivity is the sum of the change from substance A to substance B and the change from substance B to substance C, or the total number of disintegrations. This is because when we consider radioactivity, we consider disintegration so we do not consider the elements on the RHS and rather, just those on the LHS, i.e. those which are disintegrating.

(d) On solving the Eq. (1) we get Eq. (4). We solve for Eq. (2). Here the Integrating Factor is e^{bt} and the solution is given by:

$$Be^{bt} = \int_0^t aA_0e^{(b-a)t} \quad (6)$$

Upon integrating, we obtain the solution given in Eq. (5). Here as $a \ll b$, therefore, $e^{-bt} < e^{-at}$. Hence, Eq. (5) implies:

$$B = \frac{aA_0e^{-at}(1 - \frac{e^{-bt}}{e^{-at}})}{b - a}$$

As t tends to infinity the fractional term inside the bracket tends to 0 and the whole term inside the bracket tends to 1. Replacing A from Eq. (5) we get the equation of transient equilibrium:

$$\frac{B}{A} \approx \frac{a}{b - a} \quad (7)$$

The graph shown above represents how in transient equilibrium, the ratio $\frac{B}{A}$ remains constant and is equal to $\frac{a}{(b-a)}$.

(e) When $a > b$, as is the case in Fig. (4), we do

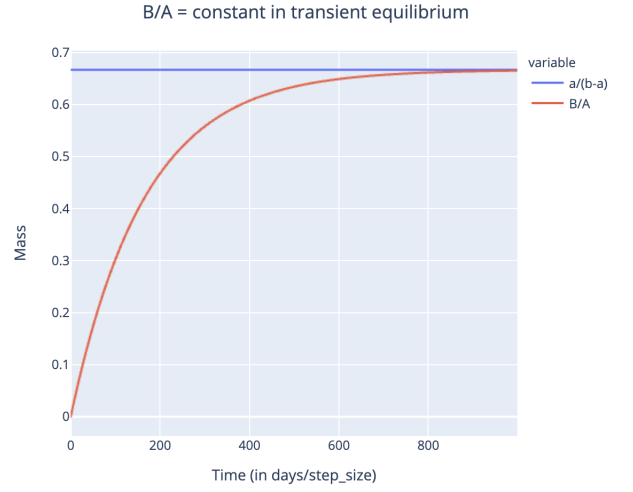


FIG. 3. Transient equilibrium: Constant ratio of Mass of B to Mass of A. Step size = 0.01 over a span of 10 days.

not observe any transient equilibrium as the ratio $\frac{B}{A}$ is not constant.

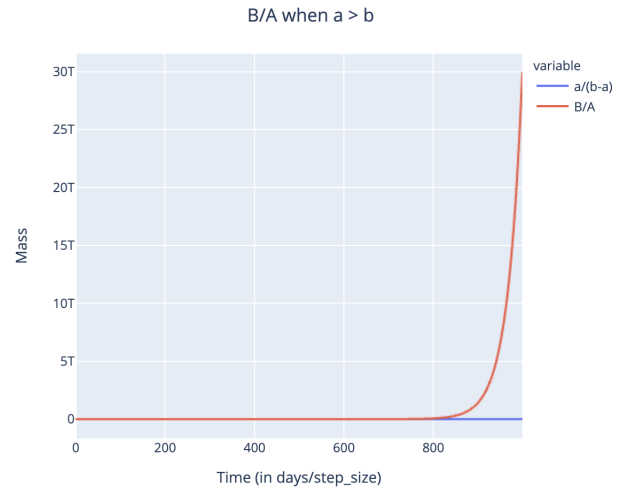


FIG. 4. When $a > b$, we do not observe transient equilibrium. Step size = 0.01 over a span of 10 days.

(f) If $a > b$ then $e^{-bt} > e^{-at}$. Following steps similar to part (d), Eq. (5) implies:

$$B \approx \frac{-aA_0e^{-bt}}{b - a} \quad (8)$$

Hence we see that the value of $\frac{B}{A}$ does not remain constant with time when $a > b$ and increases exponentially, as is seen in Eq. (8).

(g) When $a \ll b$, we have a situation known as secular equilibrium. In this situation the mass of A and B are given by the following formulae:

$$A = A_0 \quad (9)$$

$$B = \frac{aA_0}{b-a} \quad (10)$$

The mass of A and B remain almost constant. This is true because a is small, so disintegration of A is slow. There is not much change in B due to the addition of A and hence its rate remains almost constant keeping the value of B to be constant too. We try to observe this phenomena by simulating the radioactive decay of the chain:

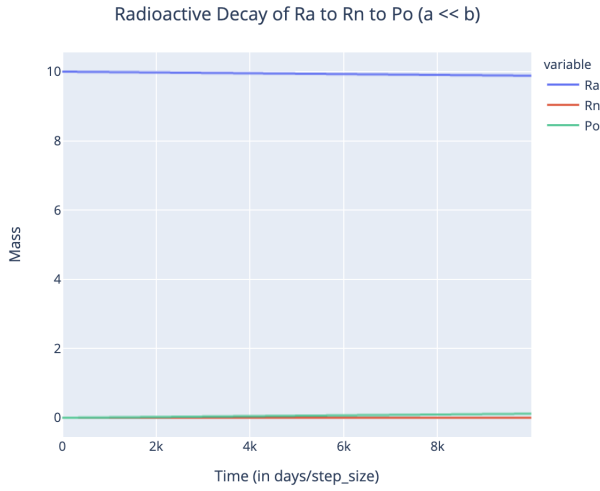
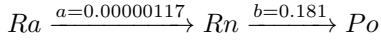


FIG. 5. Secular equilibrium: Mass of Ra and Rn remains constant. Po eventually increases in mass after a very long time, since the disintegration constant of B is small. Step size = 1 over a span of 10k days.

Here, decay rate of Ra(a) is 0.00000117 and decay rate of Rn(b) is 0.181. We see that $a \ll b$. As seen in Fig. (5) and Fig. (6), Mass of Ra and Rn remains constant with values as given in Eq. (9) and Eq. (10).

(h) When a is very small, e^{-at} approximates to almost 1 (using the Taylor series). The explanation that follows uses this. As seen in Eq. (4), when $a \ll b$, then e^{-at} tends to 1 and A tends to A_0 . Similarly from Eq. (5) we see that $e^{-bt} \ll e^{-at}$ and hence, e^{-bt} can be ignored. Hence, we get the values of A and B as given in Eq. (9) and Eq. (10).

(i) We are given a radioactive chain:

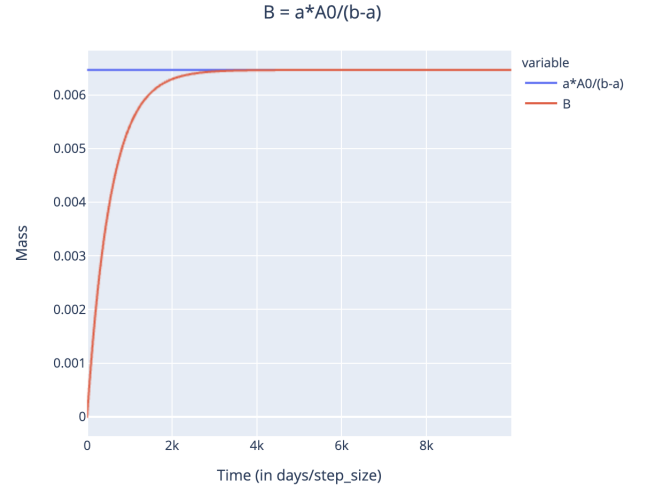
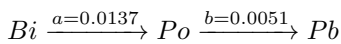


FIG. 6. Secular equilibrium: mass of Rn (B) remains constant.

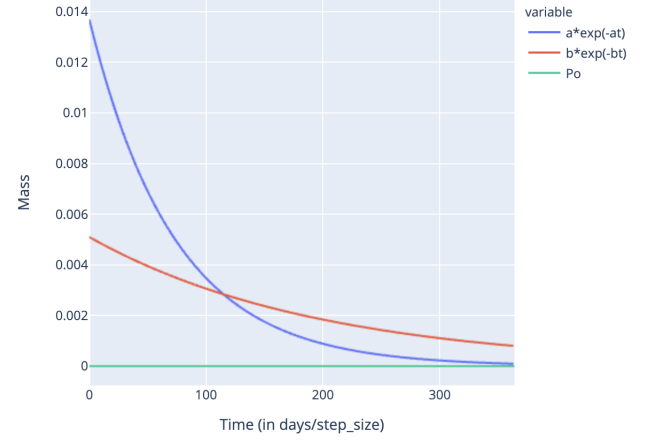


FIG. 7. Mass of Po with respect to time - the solution is found at $t = 115$ days

As seen in Fig. (7), the maximum mass of Po occurs when $t=115$ days.

(j) We try to find the time when mass of B is the maximum. Taking reference from Eq. (5), maxima occurs when

$$\frac{dB}{dt} = 0 \quad (11)$$

$$-ae^{-at} + be^{-bt} = 0 \quad (12)$$

$$\frac{a}{b} = e^{(a-b)t} \quad (13)$$

IV. CONCLUSIONS

We draw the following conclusions:

- As the disintegration constant increases in value, the maximum total radioactivity of the chain is achieved faster.
- Transient equilibrium of a three element radioactive chain is achieved when $a < b$ and in such a case, the ratio $\frac{B}{A}$ is a constant and is equal to $\frac{a}{(b-a)}$.
- Secular equilibrium of a three element radioactive chain is achieved when $a \ll b$ and in such a case, the mass of A and B remains constant and is given by Eq. (9) and Eq. (10).

$$t = \frac{\ln \frac{b}{a}}{(b-a)} \quad (14)$$

Hence,

$$B = A_0 e^{-bt} \quad (15)$$

where t is as given from Eq. (14)

(k) As seen in Fig. (7), The maximum mass of Po occurs when $t=115$ days and $ae^{-at}=be^{-bt}$. We find analytically from solving where t as given from Eq. (14) and where B (here maximum mass of Po) as given from Eq. (15) corresponds to the value we get on simulation, i.e $t=115$ days and maximum mass= 5.589n grams.

(l) We solve Eq. (14) analytically for the reaction given in part(g). Here $a=0.00000117$ and $b=0.181$. i.e. $a \ll b$. We get:

$$t = \left(\frac{\ln \frac{b}{a}}{(b-a)} \right)$$

$$t = \frac{11.94}{0.18099}$$

$$t = 65.97 \text{ days} \sim 66 \text{ days}.$$

$$\text{Mass of Rn} = 64.64 \text{ f grams}.$$

(m) As seen in Fig. (8), the maximum mass of Rn occurs when $t= 66$ days and the value matches with the value we got analytically in part (l).

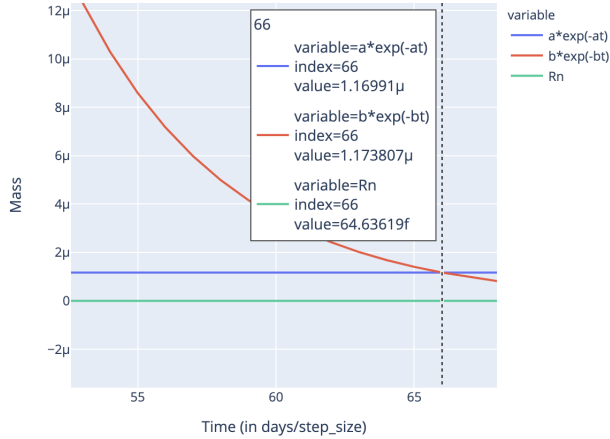


FIG. 8. Mass of Rn - peak at the solution found analytically. Step size = 1 over a span of 70 days.