

# Lab -1: Compartment Models

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In this lab, we will attempt to model the problem of system dynamics with a rate proportional to the amount of the substance. We will model and analyze the radioactive chains problem with a single compartment using numerical methods and also compare the results with its analytical solution.

## I. INTRODUCTION

Dynamic Systems are systems that change with time. In this lab we will see how compartment models can help us understand these changes. Here we have a dynamic system where the rate of change of a particular quantity is proportional to the quantity present. This can be the case when money is compounded continuously, the population change of a given species, or the radioactive decay of a substance. In this report, we will model the radioactive chains problem, with a single compartment[1].

## II. MODEL

Suppose the radioactive *substanceA* decays into substance B, and *substanceB* itself being radioactive, further decays into *substanceC*.

Let the amounts of *substanceA*, *substanceB* and *substanceC* be given by  $A$ ,  $B$ ,  $C$  respectively, and the disintegration constants of *substanceA* and *substanceB* be  $a$  and  $b$  respectively. Assume that at  $t = 0$ , *substanceB* and *substanceC* are not present in the system and the amount of *substanceA* is  $A_0$ .

Further, we are also making the following assumptions in our model. Firstly the model is homogeneous with respect to space, i.e. no notion of space has been taken under consideration in the equations, all the changes are with respect to time. Secondly, the particles of the substances are a homogeneous mixture and non-interacting within themselves or with the surroundings. Statistical fluctuations are also ignored.

Now, keeping under consideration, the aforementioned assumptions we can model the system using the following differential equations.

$$\frac{dA}{dt} = -a A \quad (1)$$

$$\frac{dB}{dt} = a A - b B \quad (2)$$

$$\frac{dC}{dt} = b B \quad (3)$$

Let us now modify the above equations and generate numerical equations to analyze the behavior of our reaction when certain parameters are altered keeping others constant.

At any given time  $t$ , the amounts of *substanceA* and *substanceB* are given by  $A$  and  $B$  respectively, let  $\Delta A$  and  $\Delta B$  be the change in the amount of *substanceA* and *substanceB* respectively and  $\Delta t$  denote the change in time  $t$ .

So to numerically analyze the differential equations we can write the equations 1, 2 and 3 as

$$\Delta A = -a A \Delta t \quad (4)$$

$$\Delta B = a A \Delta t - b B \Delta t \quad (5)$$

$$\Delta C = b B \Delta t \quad (6)$$

We simulated equations 4, 5, and 6 using Euler's method and obtained the following result.

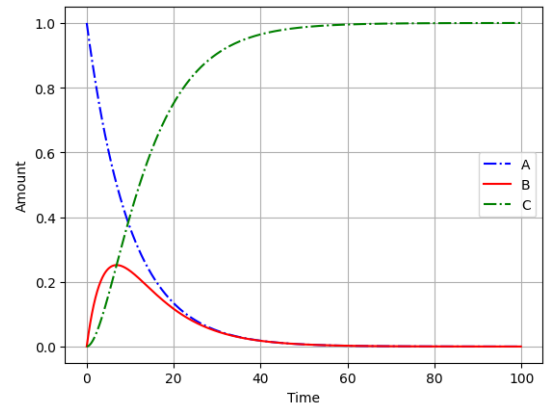


FIG. 1.  $A = 1$ ,  $a = 0.1$ ,  $b = 0.2$

Fig. 1 shows the amounts of *substanceA*, *substanceB* and *substanceC* during the time interval  $[0, 100]$  unit. Assuming the initial amounts of the substances as,  $A_0 = 1$  unit,  $B_0 = 0$  unit,  $C_0 = 0$  unit and the disintegration constants as  $a = 0.1 \text{ time}^{-1}$  and  $b = 0.2 \text{ time}^{-1}$ .

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Given the numerical solutions, we will now generate analytical solutions to our model and try to validate them empirically. Below are analytical solutions for the amounts of substances  $A(t)$ ,  $B(t)$ , and  $C(t)$  with respect to time  $t$  to make useful comparisons with our numerical solution.

On solving Eq. 1, we get,

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

$$\frac{dA}{A} = -a dt$$

$$\int_{A_0}^{A_t} \frac{dA}{A} = \int_0^t -a dt$$

Solving the above integral, we get,

$$A(t) = A_0 e^{-at} \quad (7)$$

Now, rearranging Eq. 2, and using the result from Eq. 7 we have,

$$\frac{dB}{dt} + bB = aA_0 e^{-at}$$

Solving the above equation using the Integrating Factor method, we have,  $IF = e^{bt}$ .

Multiplying the above equation by the Integrating Factor, we get,

$$e^{bt} \frac{dB}{dt} + e^{bt} bB = e^{bt} aA_0 e^{-at}$$

$$\Rightarrow \frac{d[B e^{bt}]}{dt} = aA_0 e^{-at+bt}$$

Integrating both sides of the above equation with proper limits, we get,

$$B(t) = \frac{aA_0}{b-a} \cdot (e^{-at} - e^{-bt}) \quad (8)$$

Similarly from Eq. 3 for Substance  $C$ :

$$C(t) = \frac{aA_0}{b-a} \cdot (1 - e^{-at}) \quad (9)$$

In these equations:

- $A(t)$ ,  $B(t)$ , and  $C(t)$  represent the amounts of substances  $A$ ,  $B$ , and  $C$  at time  $t$ .
- $A_0$  is the initial amount of Substance  $A$  at  $t = 0$ .
- $a$  and  $b$  are the rate constants for the reactions involving substances  $A$  and  $B$ , respectively.

### III. RESULTS

From Fig. 1, we can observe that *substanceA* decays exponentially. We will verify this observation by plotting the amount of *substanceA* on a semi-log scale. Clearly this, confirms our analytical derivation from Eq. 7.

For *substanceB*, the Fig. 1 attains a maximum value at some point and then decreases. The maximum value of *substanceB* occurs when the rate of change of *substanceB*, i.e.  $\frac{dB}{dt} = 0$ . We can say that at this point, the amount of *substanceA* that decays from  $A$  to  $B$  becomes equal to the amount of *substanceB* that decays from  $B$  to  $C$ .

Now, we will analyze the changes in the Maximum value attained by *substanceB* for different values of  $a$  and  $b$ . We will take the value of  $b$  to be constant as 0.2 and the value of  $a$  will vary from 0.1 to 10.

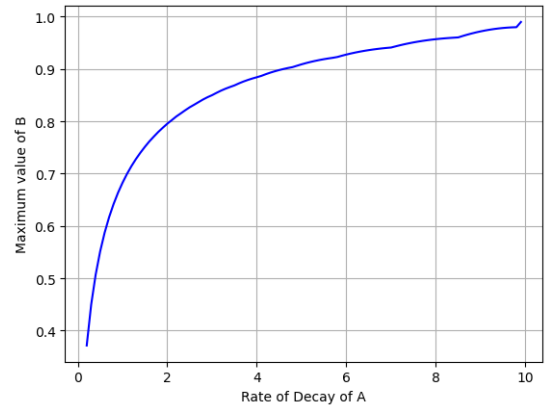
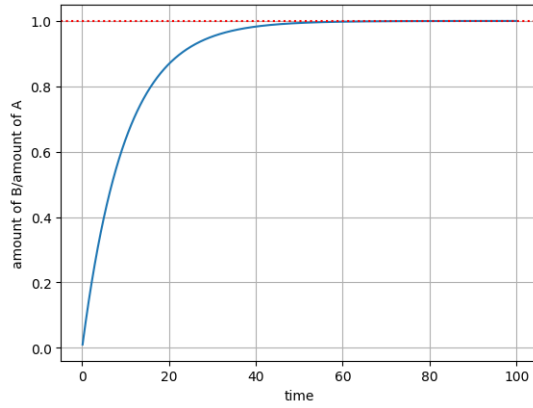


FIG. 2. Maximum amount of SubstanceB vs Rate of Decay of A

Clearly, as the value of  $a$  increases, more amount of *substanceB* gets formed, and only a small of *substanceB* gets decayed into *substanceC*. Hence, the maximum amount of *substanceB* formed increases with an increase in the value of  $a$ .

#### A. Transient Equilibrium

We first examine the case where  $a < b$ , here we observe that the ratio of the amount of *substanceB* to the amount of *substanceA* will be almost constant. Fig. 3 shows the plot between the ratio of the amount of *substanceB* to the amount of *substanceA* and time. As we can infer from Fig. 3 the ratio remains constant after  $t = 40$ .

FIG. 3.  $a = 0.1$ ,  $b = 0.2$ 

We will verify this analytically using Eq. 8

$$B(t) = \frac{aA_0}{b-a} (e^{-at} - e^{-bt}) \quad (10)$$

In the Eq. 10 since,

$$a < b \Rightarrow e^{-at} > e^{-bt}$$

hence  $\lim_{t \rightarrow \infty} e^{-bt} = 0$  so when  $t$  is large,

$$B = \frac{aA_0}{b-a} (e^{-at} - 0) \Rightarrow \frac{B}{A} \approx \frac{a}{b-a} \quad (11)$$

Since  $A = A_0 e^{-at}$  from Eq. 7

At this condition, we say that the system is in transient equilibrium.

Now let us examine the case where  $a > b$ . We observe that the ratio of the amount of *substance B* to the amount of *substance A* does not converge to a fixed number.

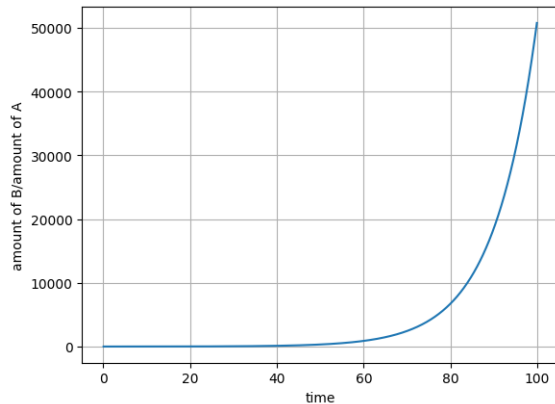
FIG. 4.  $a = 0.2$ ,  $b = 0.1$ 

Fig. 4 shows the plot between the ratio of the amount of *substance B* to the amount of *substance A* and time, which diverges as  $t$  becomes larger.

We can verify our above result analytically using Eq. 8. Since  $a > b$ , we can re-write Eq. 8 as,

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

Dividing the equation by Eq. 7, we get

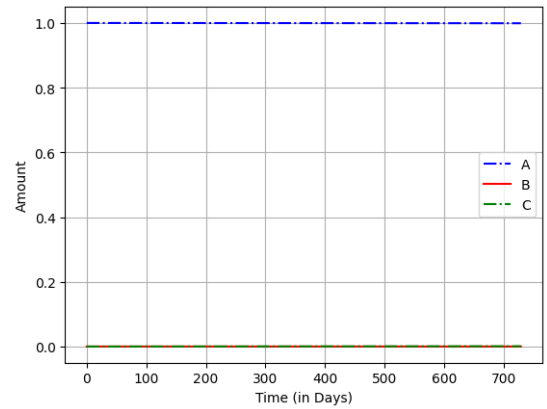
$$\frac{B}{A} = \frac{aA_0}{(b-a)(A_0 e^{-at})} (e^{-at}) - \frac{aA_0}{(b-a)(A_0 e^{-at})} (e^{-bt})$$

$$\Rightarrow \frac{B}{A} = \frac{a}{(b-a)} (1 - e^{(a-b)t})$$

Clearly from the above Eq. it will diverge as  $t$  becomes larger.

## B. Secular Equilibrium

In the previous sections, we have analysed the cases where  $a < b$  and  $a > b$ , now we will analyse the case where  $a \ll b$ . Let us take the particular example of the radioactive chain:  $Ra^{226} \rightarrow Rn^{222} \rightarrow Po^{218}$  [1]. Fig. 5 shows a numerical simulation of the chain reaction for a period of two years. We can observe the amounts of substance A, B, and C do not change i.e.  $A = A_0$  and  $B = C = 0$ .

FIG. 5.  $a \ll b$ :  $a = 0.00000117$ ,  $b = 0.181$ 

In Fig. 6, we have plotted the curve for the ratio of the amount of *substance B* to the amount of *substance A* against Time(in Days) similar to Fig. 3 and Fig. 4.

We can observe that the ratio reaches a constant value almost immediately after  $t = 0$ . This is because the rate of change disintegration of *substance A* is negligible, hence for a very long time, there is no change in the ratio.

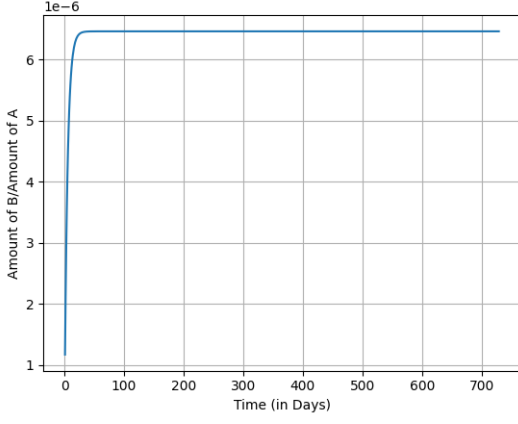


FIG. 6.  $a \lll b$  :  $a = 0.00000117$ ,  $b = 0.181$

Analytically, using Eq. 7 and Eq. 8 and as  $a \lll b$ , we can say that  $A \approx A_0$ , and  $B \approx \frac{aA_0}{b-a}$ . This condition is known as secular equilibrium. Here it appears that equilibrium is achieved, but since the amounts of *substanceA* and *substanceB* are almost constant (as in Fig. 5), we can say that the system never truly achieves equilibrium.

### C. Maximum amount of *substanceB* and the Time when maximum occurs

Let  $t = T_{max}$  be the time when *substanceB* is maximum. We know that at  $t = t_{max}$ ,  $\frac{dB}{dt} = 0$  hence, from Eq. 2 we can write

$$aA = bB \Rightarrow aA_0e^{-at} = \frac{baA_0}{(b-a)}(e^{-at} - e^{-bt}) \quad (12)$$

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

hence,

$$t_{max} = \frac{1}{a-b} \ln \frac{a}{b} \quad (14)$$

$$B_{max} = \frac{aA_0}{(b-a)}(e^{-at_{max}} - e^{-bt_{max}}) \quad (15)$$

Now we will check our analytical result by running our model, we will take the particular example of the radioactive chain:  $Bi^{210} \rightarrow Po^{210} \rightarrow Pb^{206}$  [1]. We take  $a = 0.0137da^{-1}$ ,  $b = 0.0051da^{-1}$  and the initial mass of  $Bi^{210}$ , i.e  $A_0 = 10^{-8}g$ .

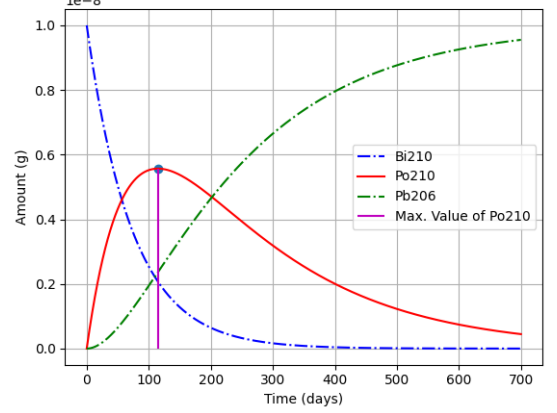


FIG. 7.  $Bi^{210} \rightarrow Po^{210} \rightarrow Pb^{206}$ ,  $a = 0.0137$ ,  $b = 0.0051$ ,  $t_{max} = 114.7$  da,  $B_{max} = 5.567730829663597e-09$  g

Similarly for the radioactive chain :  $Ra^{226} \rightarrow Rn^{222} \rightarrow Po^{218}$  [1] where  $A_0 = 1g$   $a = 0.00000117/da$  and  $b = 0.181/da$ , value of  $t_{max} = 65.4$  day and  $B_{max} = 6.4635936542996806e-06$  g.  $B_{max}$  is very small as  $a \lll b$  hence very small amount of *substanceB* will form during the reaction

## IV. CONCLUSIONS

In conclusion, we have studied the radioactive chains problem with a single compartment, where rate is proportional to the amount of substance. We have provided numerical and analytical solution to the differential equations of the model. We have analysed the model by changing various parameters and observing the values of the substances at each point of time.

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[1] A. Shiflet and G. Shiflet, *Introduction to Computational Science: Modeling and Simulation for the Sciences*, Princeton University Press, 3, 276 (2006).