Lab -1

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CS-302, Modeling and Simulation

In this lab, we analyzed a system of radioactive chain of three substances A, B, and C. A radioactively decays into B while B decays into C which is the end product of the chain. Decay rates of A and B respectively are r_a and r_b. Computational results show that regardless the value of r_a, the mass of A decreases exponentially with time and tends to zero on approaching a large enough value of time. While, the mass of substance C increases exponentially with time, the mass of substance B increases at first, becomes maximum at a certain point of time, after which it decreases and approaches zero at infinite time.

I. INTRODUCTION

The given problem represents a typical radioactive decay chain occurring in nature. For example, Radioactive lead(Pb-210) decays to non-radioactive lead(Pb-206). On the other hand, Pb-210 is replenished by decay of radium(Ra-226).

II. MODEL

We start with the assumption that at t=0 only substance A is present i.e. at t=0, m_a=m_0 and m_b=m_c=0. We also assume that the above system is completely isolated. Given the decay rates of A and B, we derive the following differential equations for rate of change of mass of each substance:

$$\dot{m_a} = -r_a \cdot m_a \tag{1}$$

$$\dot{m_b} = -r_b \cdot m_b + r_a \cdot m_a \tag{2}$$

$$\dot{m_c} = r_b \cdot m_b \tag{3}$$

$$m_A[t+1] = m_A[t] - \Delta t{\cdot}r_a{\cdot}N_A[t] \tag{4}$$

$$m_B[t+1] = m_B[t] + \Delta t(r_a{\cdot}N_A[t] - r_b{\cdot}N_B[t]) \tag{5}$$

$$m_C[t+1] = m_C[t] + \Delta t{\cdot}r_B{\cdot}N_B[t] \tag{6}$$

Eq. (1) represents the rate of change of m_a which will be equal to negative times disintegration constant r_a time the mass present of substance A m_a.

Eq. (2) represents the rate of change of m_b which will be equal to negative times disintegration constant r_b time the mass present of substance A m_b plus disintegration constant r_a time the mass present of substance A m_a.

Eq. (3) represents the rate of change of m_c which will be equal to negative times disintegration constant r_b time the mass present of substance A m_b.

Eq. (4), Eq. (5), and Eq. (6) is the system modelled using Euler's method for solving ODEs.

III. RESULTS

(b) As we can see from the model that the rate of change of m_a is negative. So we can clearly observe the monotonically decreasing curve in the graph of m_a vs. time.

As per the assumption, we know that only substance A is present initially. From the Eq. (2) we can see that initially for a certain amount of time, the rate of change of m_b is positive as m_b will be small. So, we can see the monotonous increase in starting phase. But, gradually m_b will increase as rate of change of m_b is positive. After certain amount of time, rate of change of m_b will be equal to zero as m_b increases and m_a decreases. Because of this we can see the maxima in the graph of m_b vs. time. After the maxima occurs, the curve will monotonously decrease and then finally tend to zero since the rate of change of m_b is negative.

From the Eq. (3) we can see that the rate of change of m_c is always positive. So, we can observe the monotonous increase in the curve of m_c vs. time. And the value of mass will approach the initial value of m_a.

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(c) As we can observe in Fig. 1, as the value of r_a increases, the time at which the maximum total disintegration occurs decreases.

For analysis, we iterate the decay rate of A over [0.01, 1) with time-step of 0.01. We consider decay rate of B to be 0.3. We observe that $r_a < r_b$, the time of total maximum radioactivity decreases. This behaviour is because the half-life of A decreases with increase in decay rate and hence max decomposition occurs earlier.

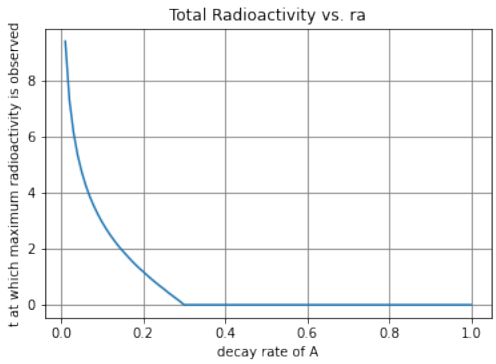

FIG. 1: Maximum Disintegration vs. Decay rate of A

(d) When $r_b > r_a$, we observe the transient equilibrium in this system as shown below in the Fig. 2.

The curve below is generated with r_a=0.1 and r_b=0.3. So, we get the equilibrium ratio equal to 0.5 according to the equation $m_b/m_a = r_a/(r_b - r_a)$, which can also be confirmed by the curve shown below in Fig. 2.

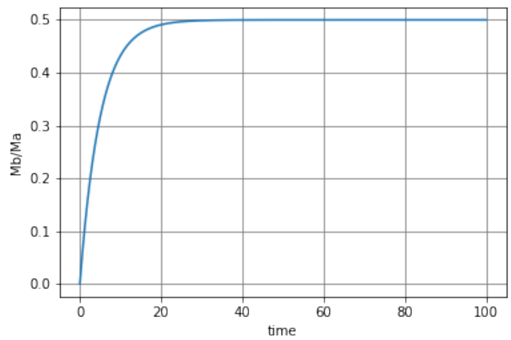

FIG. 2: Ratio of Mass of A and Mass of B vs. Time in case of transient equilibrium

(e) When $r_b < r_a$, we do not observe the transient equilibrium in the system. Fig. 3 illustrates the non-convergence using r_a=0.1 and r_b=0.03.

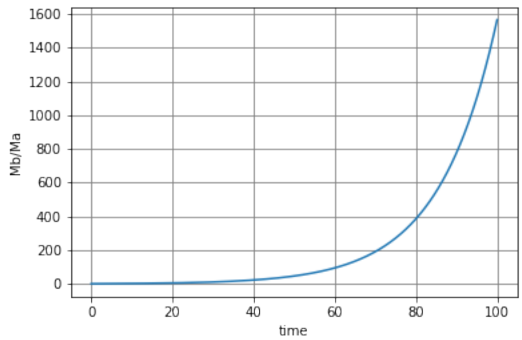

FIG. 3: Ratio of Mass of A and Mass of B vs. Time

(g) $Ra^{226} \rightarrow Rn^{222} \rightarrow Po^{218}$

Simulating the above radioactive chain with r_{Ra}=0.00000117 and r_{Rn}=0.181 for a period of one year with a time-step of bi-daily calculation, we observe secular equilibrium.

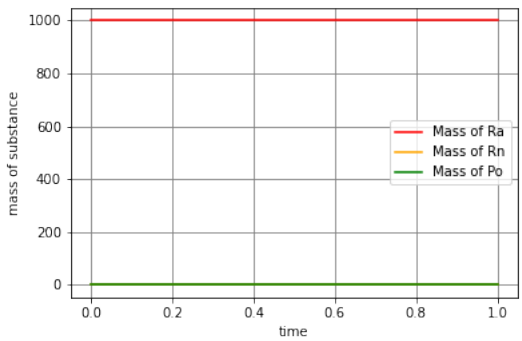

FIG. 4: Secular Equilibrium for $Ra^{226} \rightarrow Rn^{222} \rightarrow Po^{218}$

(i) $Bi^{210} \rightarrow Po^{210} \rightarrow Pb^{206}$

We simulating the above radioactive chain with r_{Bi}=0.0137, r_{Rn}=0.0051 and initial mass of Bi $M_0=10^{-8}$g for a period of 1000 years. The maximum mass observed of Po is 5.5677308e-09 g and it occurs at t=114.8 days.

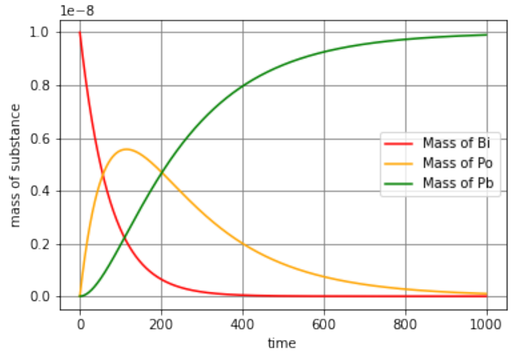

FIG. 5: Masses of substances for $Ra^{226} \rightarrow Rn^{222} \rightarrow Po^{218}$

(j) Analytically, the time at which maximum mass of B occurs, and the corresponding mass at that instant is,

$$t_B(max) = \frac{ln(\frac{b}{a})}{a-b} \tag{7}$$

$$m_B(max) = A_0 \cdot (\frac{a}{b})^{\frac{b}{b-a}} \tag{8}$$

Using Eq. (7) the time at which maximum mass of Po^{210} occurs is t=114.9days and the corresponding mass using Eq. (8) is m=5.5654955e-09 g.

(k) From our computational analysis in (i), the time at which maximum mass of Po^{210} occurs is t=114.8days and the corresponding mass is m=5.5677308e-09 g. Analytical solution has almost negligible error with respect to computational results.

(l) Using Eq. (7) the time at which maximum mass of Rn^{222} occurs is t=66 days and the corresponding mass Eq. (8) is m=0.0064635 g.

(m) In our computational results, the maximum mass occurs at t=65.6 days and the corresponding mass is m=0.0064635. The analytical solution provides almost negligible error with respect to the computational results.