Lab -1: Radioactive Decay Chain A $\rightarrow$ B $\rightarrow$ C

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MC312, Modeling and Simulation

Abstract

In this lab, we analytically and numerically study the compartment model for a radioactive decay chain: A $\rightarrow$ B $\rightarrow$ C. We explore how the system behaves for different decay rates and identify when the intermediate atom B peaks. How the changing of a & b (decay rate of A & B) affect the graphs of the quantity of the three atoms at various times? The model is solved analytically, and numerical simulations are conducted for different rate constants.

1 Introduction

Many physical systems involve cascading transformations, such as in nuclear decay or drug metabolism. In this lab, we model a sequential decay process where substance A decays into B at rate a, and B subsequently decays into C at rate b. Our goal is to understand the temporal behavior of each substance, particularly B, whose behavior is non-monotonic due to competing inflow and outflow rates.

2 Model

We consider the following system of ordinary differential equations (ODEs) to model the process:

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

$$\frac{dB}{dt} = aA - bB \tag{2}$$

$$\frac{dC}{dt} = bB \tag{3}$$

with initial conditions:

$$A(0) = A_0, \quad B(0) = 0, \quad C(0) = 0$$

Here, a and b are positive constants denoting decay rates from A to B and B to C, respectively.

3 Graph Plots

3.1 Plots of A(t), B(t) & C(t) w.r.t time:

We simulated the system of equations representing the compartment model $A \rightarrow B \rightarrow C$ using Euler's method for three sets of decay rates (a, b):

- Case 1: $a = 0.1,\ b = 1$
- Case 2: $a = 1,\ b = 0.1$
- Case 3: $a = 1,\ b = 1$

The figure below shows the time evolution of $A(t)$, $B(t)$, and $C(t)$ for each case. The results demonstrate how the intermediate quantity $B(t)$ peaks at different times depending on the relative values of a and b.

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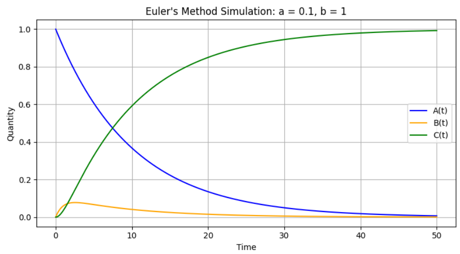
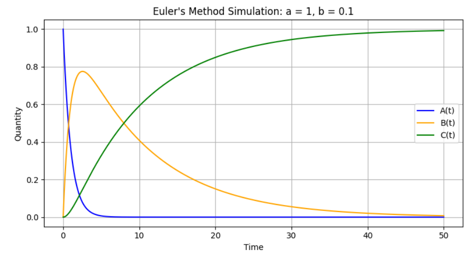
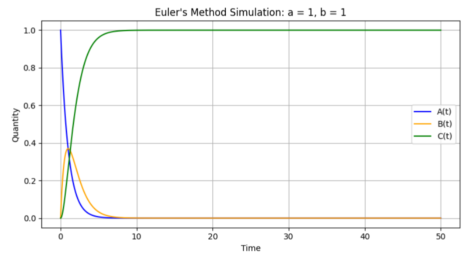


(a) Case 1: $a = 0.1,\ b = 1$



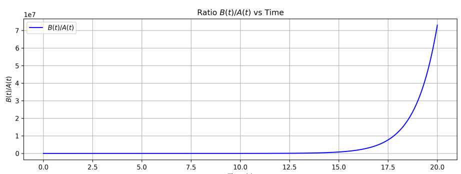
(b) Case 2: $a = 1,\ b = 0.1$



(c) Case 3: $a = 1,\ b = 1$

Figure 1: Decay simulation of $A(t)$, $B(t)$, and $C(t)$ using Euler's method for different values of a and b. In all cases: $A_0 = 1,\ B_0 = 0,\ C_0 = 0$.

3.2 Plot of $\frac{B(t)}{A(t)}$ & $\log \frac{B(t)}{A(t)}$ w.r.t time:



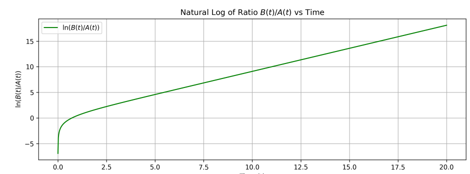


Figure 2: Plot of $\frac{B(t)}{A(t)}$ and $\log\left(\frac{B(t)}{A(t)}\right)$ over time for different decay rates. The ratio $\frac{B(t)}{A(t)}$ increases initially as B is produced from A, then decreases as B decays into C, capturing the transient peak behavior of $B(t)$.

3.3 Heatmap for the relation of the max value of B(t) and a,b:

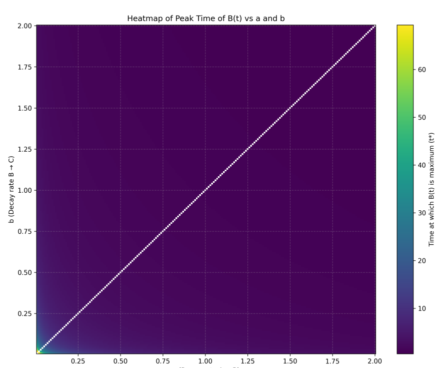


Figure 3: Heatmap showing the time t^* at which $B(t)$ reaches its maximum, as a function of decay rates a and b. The white diagonal line corresponds to $a = b$, where the general formula for t^* is undefined.

$$t^* = \begin{cases} \frac{1}{b-a} \ln\left(\frac{b}{a}\right), & \text{if } a \neq b \\ \frac{1}{a}, & \text{if } a = b \end{cases}$$

Where t^* is the value where $B(t)$ attains its maximum value.

4 Analytical Solutions

A(t):

- $\frac{dA}{dt} = -aA \quad \Rightarrow \quad A(t) = A_0 e^{-at}$

B(t):

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

Using integrating factor $\mu(t) = e^{bt}$:

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

C(t):

- $C(t) = A_0 \left[1 - \frac{be^{-at} - ae^{-bt}}{b-a}\right]$

5 Discussion of Results

5.1 Effect of decay rate relation ($a < b$ vs $a > b$):

The behavior of $B(t)$ changes significantly depending on whether $a < b$ or $a > b$:

Case	**Effect on** $B(t)$
$a < b$	B is produced slowly from A and decays quickly to C. The peak is lower and occurs later.
$a > b$	B is produced rapidly from A but decays slowly to C. The peak is higher and occurs earlier.

5.2 Equilibrium-like behavior:

When $a \approx b$, the rates of inflow (A to B) and outflow (B to C) are nearly equal. This causes $B(t)$ to temporarily remain in balance with $A(t)$, and the ratio $\frac{B(t)}{A(t)}$ stays nearly constant for some time.

5.3 Patterns and observations:

- The time t^* at which $B(t)$ peaks is very sensitive to the difference between a and b.
- As $a \to b$, the formula for t^* becomes undefined, causing a white diagonal in the heatmap. In this case, $B(t) = aA_0 t e^{-at}$ with peak at $t^* = \frac{1}{a}$.
- The heatmap clearly visualizes how t^* shifts based on the interaction between production and decay rates.