Modeling of a Radioactive Decay Chain

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1 Introduction

Radioactive decay is a fundamental process in nuclear physics, wherein unstable nuclei transform into more stable configurations through the emission of radiation. In this project, we analyze a three-component decay chain: $N_A \rightarrow N_B \rightarrow N_C$ where N_C is stable. Our goal is to solve the governing differential equations analytically and then numerically using the forward difference approximation (explicit Euler scheme). We compare the results by plotting numerical and analytical solutions for different time steps (Δt).

2 Theoretical Framework

The decay process of a radioactive nuclide is governed by a set of first-order differential equations that describe the evolution of the parent nuclide N_A, the daughter nuclide N_B, and the stable nuclide N_C. These equations form a decay chain, which we now present and solve analytically before developing a numerical approximation.

2.1 Analytical Solution

2.1.1 Parent Nuclide decay (N_A)

The parent nuclide, N_A, decays according to the first-order differential equation:

$$\frac{dN_A}{dt} = -\lambda_A N_A \tag{1}$$

where λ_A is the decay constant of the parent nuclide. This equation is separable and can be solved by integrating both sides, giving us:

$$\ln(N_A) = -\lambda_A t + C_1$$

where C_1 is a constant of integration. Applying the initial condition $N_A(0) = N_{A0}$, we determine that $C_1 = \ln(N_{A0})$. Therefore, the solution for $N_A(t)$ is:

$$N_A(t) = N_{A0} e^{-\lambda_A t} \tag{2}$$

where N_{A0} is the initial quantity of the parent nuclide.

2.1.2 Daughter Nuclide Growth and Decay (N_B)

The daughter nuclide, N_B, undergoes both production and decay, described by the following equation:

$$\frac{dN_B}{dt} = \lambda_A N_A - \lambda_B N_B \tag{3}$$

Substituting the expression for $N_A(t)$ from equation (2), we obtain:

$$\frac{dN_B}{dt} = \lambda_A N_{A0} e^{-\lambda_A t} - \lambda_B N_B \tag{4}$$

This is a linear first-order differential equation for $N_B(t)$. To solve it, we use an integrating factor, $\mu(t) = e^{\lambda_B t}$. Multiplying both sides of equation (4) by the integrating factor and integrating yields the final solution for $N_B(t)$:

$$N_B(t) = N_{B0} e^{-\lambda_B t} + \frac{\lambda_A N_{A0}}{\lambda_B - \lambda_A} \left(e^{-\lambda_A t} - e^{-\lambda_B t} \right) \tag{5}$$

2.1.3 Stable Nuclide Accumulation (N_C)

Finally, the stable nucleus N_C accumulates as the daughter nuclide decays. This is described by:

$$\frac{dN_C}{dt} = \lambda_B N_B \tag{6}$$

Integrating this equation after substituting the expression for $N_B(t)$ gives the final expression for $N_C(t)$:

$$N_C(t) = N_{C0} + N_{B0} \left(1 - e^{-\lambda_B t} \right) + \frac{N_{A0}}{\lambda_B - \lambda_A} \left[\lambda_A \left(1 - e^{-\lambda_B t} \right) - \lambda_B \left(1 - e^{-\lambda_A t} \right) \right] \tag{7}$$

2.2 Numerical Solution Using the Explicit Euler Method

The Explicit Euler method approximates the solution of ordinary differential equations using small time steps Δt. A forward difference approximation is of the form:

$$\frac{dN}{dt} \approx \frac{N(t + \Delta t) - N(t)}{\Delta t} \tag{8}$$

which rearranges to the iterative formula:

$$N(t + \Delta t) = N(t) + \Delta t \cdot \frac{dN}{dt} \tag{9}$$

Applying this scheme to our decay equations, we get the following set of iterative equations for the simulation:

$$N_A(t + \Delta t) = N_A(t) - \lambda_A N_A(t) \Delta t \tag{10}$$

$$N_B(t + \Delta t) = N_B(t) + \Delta t \left(\lambda_A N_A(t) - \lambda_B N_B(t) \right) \tag{11}$$

$$N_C(t + \Delta t) = N_C(t) + \lambda_B N_B(t) \Delta t \tag{12}$$

These equations are iterated from $t = 0$ until $t = t_{\text{final}}$ to generate the numerical approximations for N_A, N_B, and N_C.

2.3 Time of Maximum N_B

To find the time at which the concentration of N_B reaches its maximum, we differentiate the analytical solution for $N_B(t)$ with respect to time and set the derivative equal to zero. Assuming there is no initial daughter nuclide ($N_{B0} = 0$), this yields:

$$t_{\max} = \frac{\ln(\lambda_A/\lambda_B)}{\lambda_A - \lambda_B} \tag{13}$$

This expression gives the theoretical time at which N_B reaches its peak concentration.

3 Results and Analysis

3.1 Impact of Time Step (Δt) on Numerical Accuracy

This analysis investigates the accuracy of the numerical solution for $N_B(t)$ using three different time-step sizes (Δt) to assess the impact of step size on the model's accuracy compared to the analytical solution. Three step-size multipliers were chosen: coarse (1.5x), medium (1.0x), and fine (0.5x).

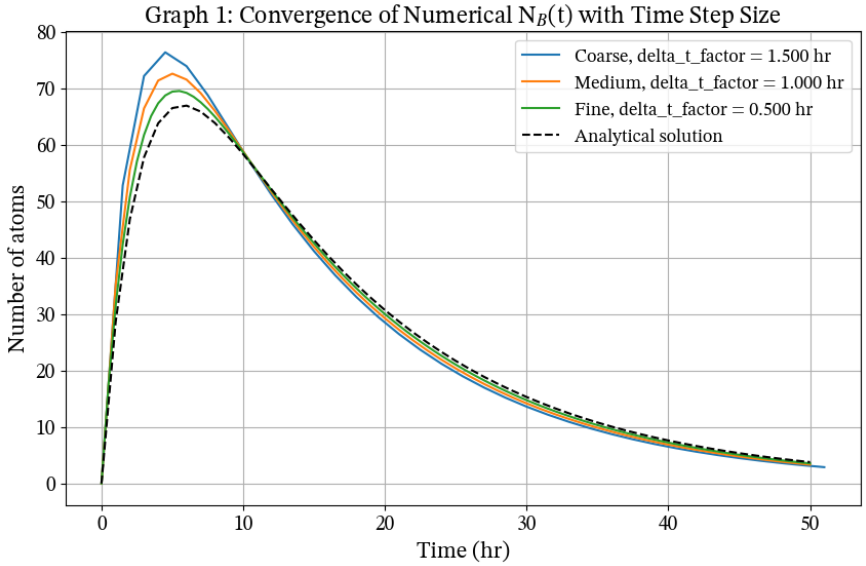

Figure 1: Comparison of the numerical solution for $N_B(t)$ at coarse, medium, and fine time steps against the exact analytical solution.

As shown in Figure 1, as the time step Δt decreases, the numerical solution converges to the analytical solution. The disparity is most evident at the peak concentration. The coarse solution overestimates the peak by 14.1%, while the fine solution is only 3.9% higher than the analytical maximum, demonstrating a clear relationship between smaller step sizes and higher accuracy.

3.2 Conservation of Total Nuclides in the System

Here, we examine the numerical solutions for all three nuclides over time and verify the conservation of the total quantity, a fundamental principle for a closed decay system. The total number of particles at any time is given by $N_{\text{total}}(t) = N_A(t) + N_B(t) + N_C(t)$, which should remain constant.

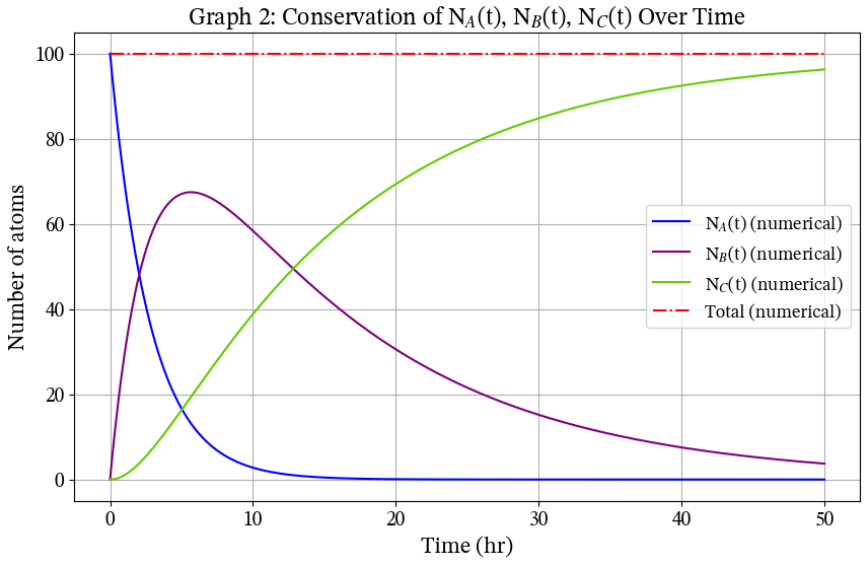

Figure 2: Numerical simulation of the concentrations of parent (N_A), daughter (N_B), and stable (N_C) nuclides over time. The total remains constant at 100.

The simulation (Figure 2) correctly models the exponential decay of N_A, the characteristic rise and fall of the intermediate nuclide N_B, and the asymptotic accumulation of the stable nuclide N_C. The sum of the three populations remained constant at the initial total of 100 throughout the simulation, confirming that the numerical model respects the law of conservation.

3.3 Convergence of the Time of Maximum Daughter Nuclide ($t_{\max}$)

This final analysis investigates how the numerically computed time of maximum N_B concentration, $t_{\max}$, varies with Δt. We expect the numerical $t_{\max}$ to converge to the analytical value derived in equation (13) as the time step Δt approaches zero.

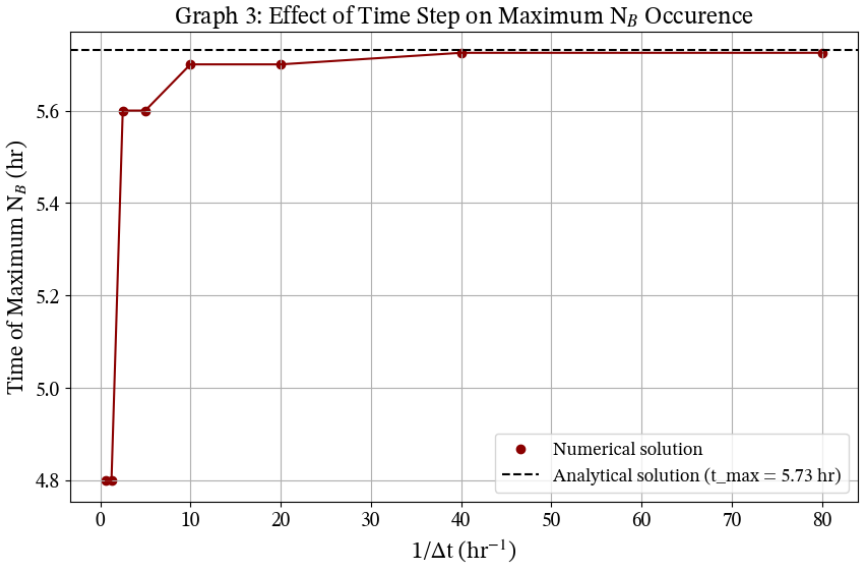

Figure 3: Convergence of the numerical $t_{\max}$ to the analytical solution (dashed line) as the time step Δt decreases (plotted as $1/\Delta t$).

Figure 3 shows that as $1/\Delta t$ increases (i.e., Δt gets smaller), the numerical values of $t_{\max}$ converge to the analytical solution ($t_{\max} = 5.73$ hr). This result confirms that our numerical method behaves as expected, with accuracy improving significantly as the simulation's temporal resolution increases. This highlights the classic trade-off between computational cost and accuracy in numerical simulations.

4 Conclusion

The analytical and numerical solutions to the three-component decay chain were successfully implemented and compared. The numerical solutions, based on the Explicit Euler method, converged to the analytical results as the time step Δt decreased, demonstrating the model's accuracy. Key physical properties, such as the time of maximum daughter nuclide concentration and the conservation of total particles, were verified with both approaches, confirming theoretical predictions and validating the simulation.