Analysis and Computational Foreword-Difference Approximation Method for Solving Three-Component Nuclear Decay Chains

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1 Theory

1.1 Differential Equation and Analytical Solution for the First Isotope

The decay of radioactive materials is widely known to use a first order rate equation shown in *Equation 1* [1] where N is the quantity of the radioactive isotope, λ represents the decay constant, and t represents time.

$$\frac{dN}{dt} = -\lambda N \tag{1}$$

The decay constant λ is derived from the half life value $t_{1/2}$ which represents the amount of time it takes for a particular isotope to decay into half of it's original mass. This relation is expressed in *Equations 2 and 3* [2].

$$t_{1/2} = \frac{ln(2)}{\lambda} \tag{2}$$

$$\lambda = \frac{ln(2)}{\lambda} \tag{3}$$

Since half-lives are in general known values for an isotope, the decay constants are therefore known values and *Equation 1* can be used to model decay chains. For the first component in a decay chain with decay constant λ_A, N_A can be analytically solved for due to *Equation 1* being separable. The solution is then *Equation 4* where N_0 represents the initial quantity of the isotope.

$$N_A = N_0 e^{-\lambda_A t} \tag{4}$$

1.2 Differential Equation and Analytical Solution for the Second Isotope

The second component of the decay chain has two parts: the amount being created from a decaying first component and the decay it undergoes itself. Therefore the rate of change associated with the quantity of the second component is *Equation 5* where λ_B is the decay constant of the second component and B_0 is the initial quantity of the second component.

$$\frac{dN_B}{dt} = \lambda_A N_A - \lambda_B N_B \tag{5}$$

The $\lambda_A N_A$ part of the equation denotes the contribution from the decaying isotope A and the $-\lambda_B N_B$ part denotes the decay that isotope B undergoes. This is a first order linear equation that may be solved with the use of integrating factor yielding *Equation 6* [3].

$$N_B = \frac{\lambda_A}{\lambda_B - \lambda_A} N_{A_0}(e^{-\lambda_A t} - e^{-\lambda_B t}) + N_{B_0} e^{-\lambda_B t} \tag{6}$$

The first part of this equation denotes how much of isotope B has decayed from isotope A and takes into consideration that this quantity is also in the process of decaying. The other part of the equation denotes the initial concentration of isotope B which is also decaying.

1.3 Differential Equation and Analytical Solution for the Third Isotope

For the last isotope in our three-isotope decay chain, we should assume that it is not decaying as it is the final step in the decay chain. Because of this, the only contribution to the change of quantity of this isotope is the amount that has decayed from the previous one, a notion represented in *Equation 7*.

$$\frac{dN_C}{dt} = \lambda_B N_B \tag{7}$$

While using *Equation 6* for N_B and solving this equation analytically is possible, it is easier to think about the concept intuitively and take advantage of the principle that there is a finite unchanging amount of substance in the system. Because of this fact we know that the amount of Isotope C is equal to the initial total amount of each isotope minus what is contained in Isotope A and what is contained in Isotope B at a given time. Putting this together yields *Equation 8*.

$$N_C = (N_{A_0} + N_{B_0} + N_{C_0}) - (\frac{\lambda_A}{\lambda_B - \lambda_A} N_{A0}(e^{-\lambda_A t} - e^{-\lambda_B t}) + N_{B_0} e^{-\lambda_B t}) - (N_{A_0} e^{-\lambda_A t}) \tag{8}$$

1.4 Derivation of Numerical Solution

Along with the analytical solutions, numerical methods may be employed to solve these differential equations. The forward difference approximation method was employed in solving these equations. This method is outlined in *Equation 9* [4].

$$\frac{df}{dt}(x) = \frac{f(x + h) - f(x)}{h} \tag{9}$$

In the context of using this as a computational method for solving differential equations, it is most useful to solve this equation for $f(x+h)$ as it is in *Equation 10* so that we may use it to fill an array with values based on the initial value. An example of what this would look like for the first isotope using *Equation 1* for $\frac{df}{dt}$ is shown in *Equation 11*.

$$f(x + h) = \frac{df}{dt}(x) * h + f(x) \tag{10}$$

$$f(i + \delta t) = -\lambda_A N_A[i]\delta t + N_A[i] \tag{11}$$

1.5 Derivation of Time of Maximum of Second Isotope

To solve for the maximum value of isotope B, we can employ the fact that all critical points occur when the derivative is equal to zero. Since there is only one critical point on the decay path of isotope B, we know that is the maximum. To solve for that critical point, we can then take *Equation 5* and set the left side of the equation equal to zero as done in *Equation 12*. The maximum concentration of N_B can then be solved as is done in *Equation 13*.

$$0 = \lambda_A N_A - \lambda_B N_B \tag{12}$$

$$N_B = \frac{\lambda_A N_A}{\lambda_B} \tag{13}$$

We can then substitute *Equation 4* for N_A and *Equation 6* for N_B to get an equation that may be solved for t. Algebraically, this is a difficult task and so by moving everything to one side of the equation (*Equation 14*), we can use SymPy to solve the equation for us (*Equation 15*).

$$0 = \frac{\lambda_A N_{A_0} e^{-\lambda_A t}}{\lambda_B} - \left(\frac{\lambda_A}{\lambda_B - \lambda_A} N_{A_0}(e^{-\lambda_A t} - e^{-\lambda_B t}) + N_{B_0} e^{-\lambda_B t}\right) \tag{14}$$

$$t = \frac{-ln(\lambda_B \frac{N_{A_0}\lambda_A + N_{B_0}\lambda_A - N_{B_0}\lambda_B}{N_{A_0}\lambda_A^2})}{\lambda_A - \lambda_B} \tag{15}$$

2 Results

2.1 Numerical Solution with Different Δt's

Calculations in the results section are based values: $t_{1/2_A} = 2.53 hrs$, $t_{1/2_B} = 11.05 hrs$, N_{A_0}, N_{B_0}, N_{C_0}, $t_{final} = 60 hrs$, $\Delta t = 1$. These values are able to be altered and the values may be still be calculated with the associated program. The Numerical solutions are calculated using the method outline in *Equation 11*. There are three variations of the numerical solution. The coarse numerical solution uses the Δt above. The medium numerical solution uses half that value so there are double the amount of points and the graph is more precise. The fine numerical solution uses a quarter of the original Δt and therefore has the most points and is the most precise. The analytical solutions found in *Equations 4,6, and 8* are plotted with these numerical solutions in *Figure 1*.
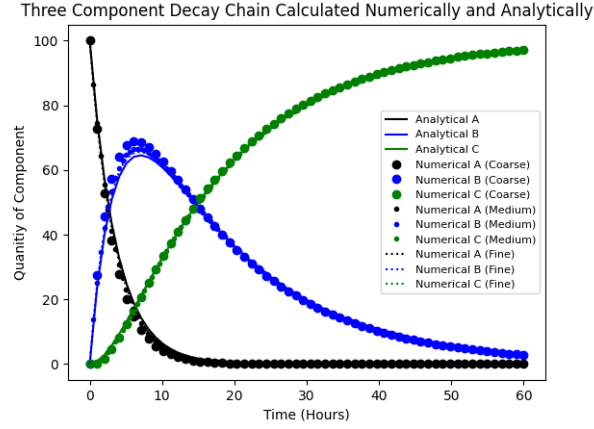
Figure 1: Graph of Coarse, Medium and Fine Numerical Solutions for Isotopes A, B, and C along with Analytical Solution

2.2 Numerical Solutions and the Sum of Isotopes over Time

Since radioactive decay is a mass-conserving process. The sum of all isotopes at any given time should be constant. To test this, the most accurate of the numerical calculations (fine) for each isotope were plotted with the sum of every isotope at every time value. The results in *Figure 2* demonstrate this fact.
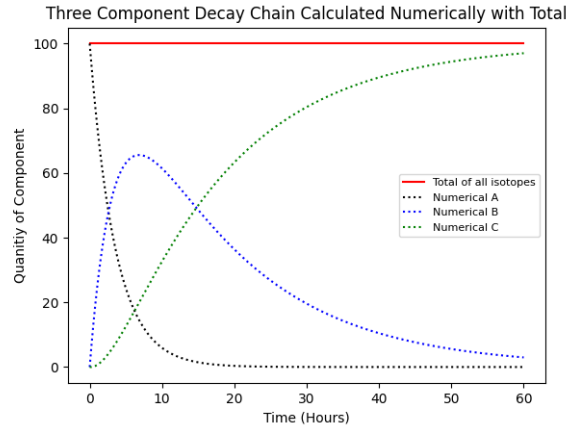

Figure 2: Graph of Fine Numerical Solutions along with Sum of All Isotopes at Every Time Value

2.3   Time Maximum of Second Isotope

Solving for the time at which N_B is at it's maximum can be done via the method described in *Equation 15* for the analytical solution to get *Equation 16*.

$$t = 6.97875 hrs \tag{16}$$

However, from *Figure 1* a pattern can be identified in the numerical solutions. As Δt gets smaller, the time of maximum N_B increases approaching the analytical value. This phenomena is demonstrated in *Figure 3* where different values of $\frac{1}{\Delta t}$ are plotted against the time at which N_B is at a maximum. It is clear from this plot that as the calculations get finer (e.g. lower Δt and therefore, more points) they get more precise and the time approaches the analytical value.
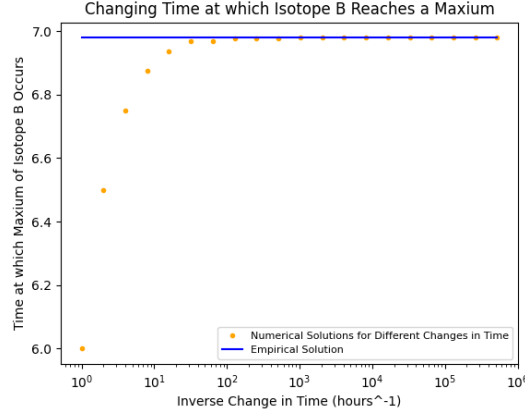
Figure 3: Graph Comparing the Effects of Different Changes in Time with the Time at which Isotope B Reaches a Maximum

References

[1] P. Amodio, Y. Blinkov, Vladimir Gerdt, and R. Scala. On consistency of finite difference approximations to the navier-stokes equations. *Lecture Notes in Computer Science*, pages 46–60, Jan. 2013.

[2] Boston University. Radioactivity, 2024. Accessed: Feb. 26, 2024.

[3] E. E. Lewis. *Fundamentals of Nuclear Reactor Physics*. 2008.

[4] Purdue University. Half_life, Unknown. Accessed: Feb. 26, 2024.